1 Ein rafeind innilokuð í kúlu með geisla a

Bylgjuföllin eru

$$\psi_{n\ell m}(r,\theta,\varphi) = A_{n\ell}\, j_\ell\left(\frac{\beta_{n\ell} r}{a}\right) Y_{\ell m}(\theta,\varphi)$$

Eigingildi H eru

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2 = E_1 \beta_{n\ell}^2$$

$$ka = \sqrt{\frac{2ma^2}{\hbar^2}E} = \sqrt{\frac{E}{E_1}} = \beta_{n\ell}$$: n-ta núllstöð kúlu Bessel falls ℓ

$n = 1, 2, \ldots\ldots$

Viljum finna ástönd samsvarandi við 1s, 2s og 2p-ástönd vetnisatóms.

1s í vetni engin núllstöð, hér er þá ein núllstöð
$l=0$, $m=0$
á jaðri samsvarandi ástand, $l=0$, $m=0$
$n=1$

2s í vetni ein núllstöð, hér eru þá tvær núllst.,
$l=0$, $m=0$
ein á jaðri $n=2$, $l=0$, $m=0$

2p í vetni engin núllstöð, hér er þá ein núllstöð,
$l=1$, $m=-1,0,+1$
$n=2$
á jaðri $n=1$, $l=1$, $m=-1,0,+1$, og önnur í $x=0$

1s

$$\psi_{100}(r,\theta,\varphi) = A_{10}\, j_0\left(\frac{\beta_{10} r}{a}\right) Y_{00}(\theta,\varphi)$$

$$j_0\left(\frac{\beta_{10} r}{a}\right) = \frac{\sin\left(\frac{\beta_{10} r}{a}\right)}{\left(\frac{\beta_{10} r}{a}\right)}$$

fallið $\sin(x)/x$ hefur enga núllstöð í $x = 0$, fyrsta núllstöðin er $x = \pi$. Setjum á jaðar

$\rightarrow r = a$ og $\beta_{10} = \pi$

$$\rightarrow E_{10} = E_1 \pi^2 , \quad E_1 = \frac{\hbar^2}{2ma^2}$$

2s

$$\psi_{200}(r,\theta,\varphi) = A_{20}\, j_0\left(\frac{\beta_{20} r}{a}\right) Y_{00}(\theta,\varphi)$$

Sama r-fall næsta núllstöð

$$r = a \quad \longrightarrow \quad \beta_{20} = 2\pi$$

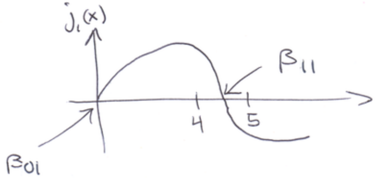
$$\longrightarrow \quad E_{20} = E_1 \, (2\pi)^2 = 4 \cdot E_{10}$$

2p

$$\Psi_{110}(r,\theta,\varphi) = A_{11} \, j_1\left(\frac{\beta_{11} r}{a}\right) Y_{1m}(\theta,\varphi)$$

$$m = -1, 0, +1$$

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$$



$r = a$ og $\beta_{11} = 4.4934$

$$\longrightarrow E_{11m} = E_1 \, \beta_{11}^2$$

⑤

þannig að ↙ 2s og 2p hafa mism. orku

$$2s: \quad E_{20} = 4 \cdot E_{10}$$

$$2p: \quad E_{11m} = E_1 \beta_{11}^2 = \frac{E_{10}}{\pi^2} \beta_{11}^2 \approx 2.0457 \cdot E_{10}$$

Fyrir vetnisatóm fékkst

$$E_n = -\frac{R_y}{n^2}$$

$E_1 = -R_y$ 1s

$E_2 = -\frac{R_y}{4}$ 2s, 2p

(6)

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a) Sannreyna

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

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

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

fyrir

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Eg reyni octave

sz = [1/2, 0 ; 0, -1/2]

sx = [0, 1/2 ; 1/2, 0]

sy = [0, -i/2 ; i/2, 0]

$$sx*sy - sy*sx = \begin{pmatrix} i/2 & 0 \\ 0 & -i/2 \end{pmatrix}$$

$$= i S_z$$

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

$$Sy * Sz - Sz * Sy = \begin{pmatrix} 0 & i/2 \\ i/2 & 0 \end{pmatrix} = i S_x$$

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

$$Sz * Sx - Sx * Sz = \begin{pmatrix} 0 & 1/2 \\ -1/2 & 0 \end{pmatrix} = i S_y$$

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

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b) sýna að

$$\sigma_j \sigma_k = \delta_{jk} + i \sum_l \epsilon_{jkl} \sigma_l$$

Munnið

$$S_x = \frac{\hbar}{2}\sigma_x$$

$$S_y = \frac{\hbar}{2}\sigma_y$$

$$S_z = \frac{\hbar}{2}\sigma_z$$

Nota octave aftur

Byrja að sannreyna að

$$(\sigma_i)^2 = \mathbb{1} \quad \text{fyrir } i = x, y, z$$

$$\epsilon_{iil} = 0$$

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

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

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

passar við $\sigma_j\sigma_k = \delta_{jk} + i\sum_l \epsilon_{jkl}\sigma_l$