(1)

Athugum $|n, n-1, m\rangle$ -ástand vetnisatóms

Samkvæmt fyrirlestri og bók er almenna bylgjufallið

$$\psi_{n\ell m}(\vec{r}) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]}}\, e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na}\right) Y_{\ell m}(\theta,\phi)$$

Ef $\ell = n-1$, (hæsta leyfilega ℓ-gildi ástands með n)

þá er Laguerre $L_0^{2n-1}\left(\frac{2r}{na}\right) = 1$

því $2\ell+1 = 2n-1$ og $n-\ell-1 = 0$

Ég nota aðra skilgreiningu á Laguerre en bókin,

$$L_n^{\alpha}(x) = e^{x}\frac{x^{-\alpha}}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^{n+\alpha}\right)$$

$$\psi_{n,n-1,m}(\vec{r}) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n[(2n-1)!]}}\, e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{n-1} Y_{n-1,m}(\theta,\phi)$$

sjá http://en.wikipedia.org/Laguerre-polynomials

eða Lebedev. N.N., Dover

a) Athugum stöðluninna

$$\int_0^\infty r^2 dr\, d\Omega\, \left|\psi_{n,n-1,m}(\vec{r})\right|^2$$

$$= \left(\frac{2}{na}\right)^3 \frac{1}{2n\left[(2n-1)!\right]} \int_0^\infty r^2 dr\; e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \left(\frac{2}{na}\right)^3 \frac{n^3 a^3}{2n\left[(2n-1)!\right]\, 8} \int_0^\infty \left(\frac{2r}{na}\right)^2 d\left(\frac{2r}{na}\right) e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \frac{1}{2n\left[(2n-1)!\right]} \int_0^\infty du\; u^{2n} e^{-u} = \frac{\Gamma(2n+1)}{2n\left[(2n-1)!\right]} = 1$$

b) Reiknið væntigildin fyrir $\langle r \rangle$ og $\langle r^2 \rangle$

$$\langle r^p \rangle = \int_0^\infty r^{2+p}\, dr\, d\Omega\, \left|\psi_{n,n-1,m}(\bar{r})\right|^2$$

$$= \left(\frac{2}{na}\right)^3 \frac{1}{2n(2n-1)!} \int_0^\infty r^{2+p}\, dr\, e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n-2}$$

$$= \left(\frac{2}{na}\right)^3 \frac{n^3 a^3}{2n(2n-1)! \cdot 8} \frac{(na)^p}{2^p} \int_0^\infty d\left(\frac{2r}{na}\right) e^{-\frac{2r}{na}} \left(\frac{2r}{na}\right)^{2n} \left(\frac{2r}{na}\right)^p$$

$$= \left(\frac{na}{2}\right)^p \frac{1}{(2n)!} \int_0^\infty du\, e^{-u}\, u^{2n+p}$$

$$\langle r\rangle = \left(\frac{na}{2}\right)\frac{1}{(2n)!}\int_0^\infty du\, e^{-u}\, u^{2n+1} = \frac{na}{2}\,\frac{\Gamma(2n+2)}{(2n)!}$$

$$= \frac{na}{2}(2n+1) = na\left(n+\frac{1}{2}\right)$$

$$\langle r^2\rangle = \left(\frac{na}{2}\right)^2\frac{1}{(2n)!}\int_0^\infty du\, e^{-u}\, u^{2n+2} = \left(\frac{na}{2}\right)^2\frac{\Gamma(2n+3)}{(2n)!}$$

$$= \left(\frac{na}{2}\right)^2(2n+1)(2n+2) = (na)^2\left(n+\frac{1}{2}\right)(n+1)$$

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c) $$\sigma_r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = na\sqrt{\left\{\left(n+\tfrac{1}{2}\right)(n+1) - \left(n+\tfrac{1}{2}\right)^2\right\}}$$

$$\sigma_r = (na)\sqrt{\left(n+\tfrac{1}{2}\right)} \cdot \frac{1}{\sqrt{2}}$$

$$\rightarrow \quad \sigma_r / \langle r \rangle = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{n+\frac{1}{2}}} = \frac{1}{\sqrt{2n+1}}$$

$\langle r \rangle \sim n^2 \cdot a \quad \rightarrow$ fjarlægð rafeindar vex sem n^2

en $\dfrac{\sigma_r}{\langle r \rangle} = \dfrac{1}{\sqrt{2n+1}}$ þýðir að bylgjufallið

þrengist með vaxandi n

$\rightarrow$ stefnir á klassíska braut

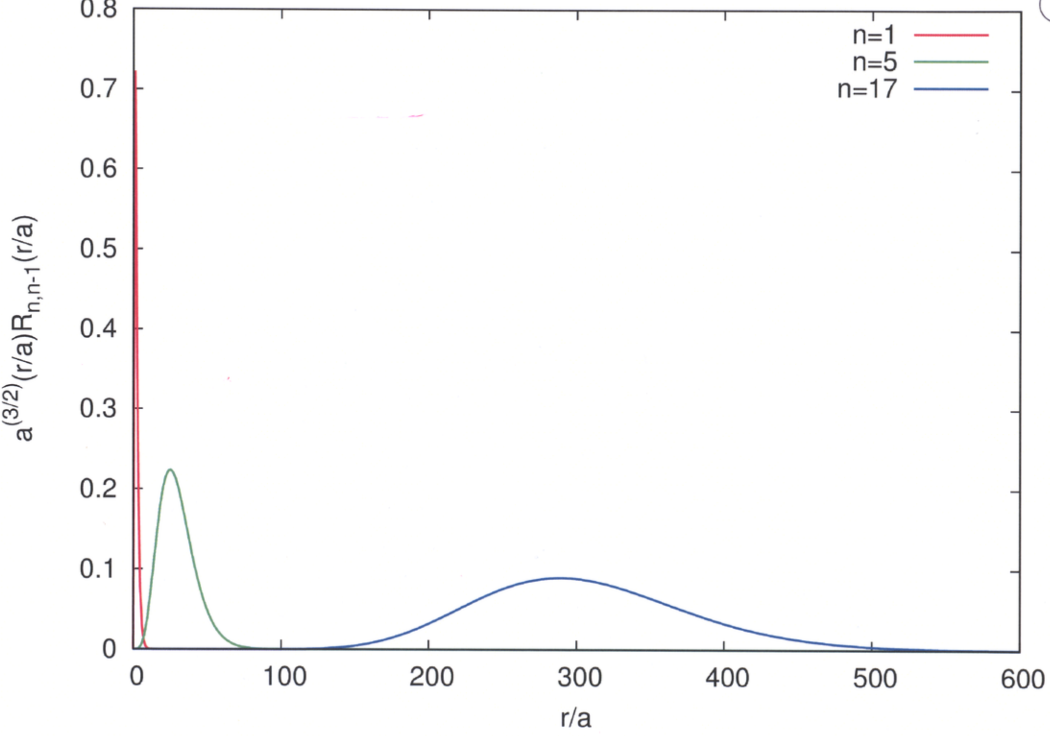
d) Teikna fyrir $n = 1, \; 5, \; 17$

$$R_{n,n-1}(r) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n(2n-1)!}}\; e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^{n-1}$$

$$R_{n,n-1}\left(\frac{r}{a}\right) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{1}{2n(2n-1)!}}\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)} \left(\frac{r}{a}\right)^{n-1} \cdot \left(\frac{2}{n}\right)^{n-1}$$

$$a^{3/2}\left(\frac{r}{a}\right) R_{n,n-1}\left(\frac{r}{a}\right) = \left(\frac{2}{n}\right)^{n-1} \sqrt{\left(\frac{2}{n}\right)^3 \frac{1}{2n(2n-1)!}}\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)} \left(\frac{r}{a}\right)^{n}$$

$$a^{3/2}\left(\frac{r}{a}\right) R_{n,n-1}\left(\frac{r}{a}\right) = F(n)\; e^{-\frac{1}{n}\left(\frac{r}{a}\right)} \left(\frac{r}{a}\right)^{n}$$



n=1
n=5
n=17
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
100
200
300
400
500
600
r/a
a^(3/2)(r/a)R_{n,n-1}(r/a)

② Finna fylkja-útsetningu S_y og S_z fyrir eind með spuna $3/2$ í grunni eiginástanda S_z

S_z hefur eiginástöndin

$$\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle \quad \left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle$$

Notum (4.136): $S_\pm |s,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}\,|s,m\pm 1\rangle$

og $S_y = \frac{1}{2i}\left(S_+ - S_-\right)$

$$S_+\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = 0$$

$$S_+\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle = \hbar\sqrt{\tfrac{3}{2}\cdot\tfrac{5}{2}-\tfrac{1}{2}\cdot\tfrac{3}{2}}\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle$$

$$S_+\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle = 2\hbar\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},+\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle$$

$$S_+\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},+\tfrac{1}{2}\right\rangle = 2\hbar\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle$$

$$S_-\left|\tfrac{3}{2},-\tfrac{1}{2}\right\rangle = \sqrt{3}\,\hbar\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle \qquad S_-\left|\tfrac{3}{2},-\tfrac{3}{2}\right\rangle = 0$$

$$\rightarrow S_+ = \hbar\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$S_- = \hbar\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$S_y = \frac{1}{2i}\left(S_+ - S_-\right)$$

$$= \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{pmatrix}$$

Eigingildi S_y

Reynt ~~við~~ octave getur

$$+\frac{\hbar}{2}\cdot 3$$

eins og ~~við~~ mátti búast

$$+\frac{\hbar}{2}\cdot 1$$

$$-\frac{\hbar}{2}\cdot 1$$

$$-\frac{\hbar}{2}\cdot 3$$