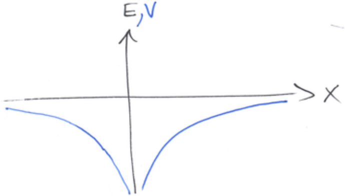
Vetnisatómið

Rafstöðumódel +e punkthleðslu (líkan af kjarnanum með sinni róteind)

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$



Dreifilausnir með $E>0$

Bundnar lausnir með $E<0$

Bundin ástönd

$$-\frac{\hbar^2}{2m} d_r^2 u(r) + \left[-\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 l(l+1)}{2mr^2}\right] u = Eu$$

Setjum $\kappa = \frac{\sqrt{-2mE}}{\hbar}$

$$\frac{1}{\kappa^2} d_r^2 u = \left\{1 - \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa}\frac{1}{(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2}\right\} u$$

$$\frac{1}{\kappa^2} d_r^2 u = \left\{1 - \frac{2}{(\kappa a)(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2}\right\} u$$

$$\boxed{a = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.529 \cdot 10^{-10}\,\mathrm{m}}$$

Bohr geisli

Náttúrulegur lengdarskali

skiptum um breytistærð

$$\rho = \kappa r\,, \quad \rho_0 = \frac{2}{a\kappa}$$

$$\rightarrow d_\rho^2 u = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u$$

Aðfellulausnir

$\rho \rightarrow \infty$ þá eru stærstu liðirnir

$$d_\rho^2 u \approx u$$

með lausn

$$u(\rho) = Ae^{-\rho} + Be^{\rho}$$

Normanleiki $\rightarrow$ $B = 0$

$$u(\rho) \sim Ae^{-\rho}$$

$\rho \rightarrow 0$

$$d_\rho^2 u \approx \frac{l(l+1)}{\rho^2} u$$

með almennri lausn

$$u(\rho) = C\rho^{l+1} + D\rho^{-l}$$

normanleiki $\rightarrow$ $D = 0$

$$\rightarrow u(\rho) \sim C\rho^{l+1}$$

Reynum því lausnaformin

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

Radial jafnan verður þá

$$\rho\, d_\rho^2 v + 2(l+1-\rho)\, d_\rho v + (\rho_0 - 2(l+1))\, v = 0$$

Lausn jöfnunar án sérstöðupunkts í $\rho = 0$ er

$$v(\rho) = \Phi\left(l+1-\frac{\rho_0}{2},\ 2l+2;\ 2\rho\right)$$

Φ er hypergeometrísta confluent fallið

það mun ekki geta staðbundin lausn nema

$$l+1-\frac{\rho_0}{2} \text{ sé neikvæð heiltala eða } 0$$

$$\to \quad l+1-\frac{\rho_0}{2} = -n_r \qquad (*)$$

þar sem n_r er radial skammtatala með

$n_r = 0, 1, 2, 3, \ldots$

þegar (*) er uppfyllt
verður fallið Φ að
endanlegri margliðu

$$L_{n_r}^{2l+1}(2\rho) = \binom{n_r + 2l+1}{n_r} \Phi(-n_r, 2l+2, 2\rho)$$

þar sem $L_{n_r}^{2l+1}(2\rho)$ eru margliður
Laguerre (associated)

$L_0^0 = 1$

$L_1^0 = -x+1$

$L_2^0 = x^2-4x+2$

$L_0^2 = 2$

$L_1^2 = -6x+18$

$\vdots$

(*) gefur líka orkurófið

$$l + 1 - \frac{\rho_0}{2} = -n_r$$

$$\underbrace{n_r + l + 1}_{} = \frac{\rho_0}{2}$$

heiltala, köllum hana n
aðal skammtatalan n

$$n = n_r + l + 1$$

$$n = \frac{\rho_0}{2} = \frac{1}{a\kappa}$$

$$\to n^2 = \frac{1}{a^2\kappa^2}$$

$$\to \kappa^2 = \frac{1}{a^2 n^2}$$

$$\kappa^2 = -\frac{2mE}{\hbar^2}$$

$$\to -\frac{2mE}{\hbar^2} = \frac{1}{a^2 n^2}$$

$$\to E = -\frac{\hbar^2}{2ma^2}\frac{1}{n^2}$$

eða

$$\boxed{E_n = -R_y \cdot \frac{1}{n^2} \qquad n = 1, 2, 3, 4, \dots \quad n \in \mathbb{N}}$$

$$R_y = \frac{\hbar^2}{2ma^2} = \frac{\hbar^2}{2m}\frac{m^2e^4}{(4\pi\epsilon_0\hbar^2)^2}$$

$$= \frac{me^4}{\hbar^2 32\pi^2\epsilon_0^2} = \frac{me^4}{8h^2\epsilon_0^2}$$

$$\boxed{R_y = -13.6\ eV}$$

fyrir rafeind í tómarúmi

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

Eiginföllin eru kornrétt

$$\int r^2 dr \sin\theta d\theta d\phi\; \psi^*_{n\ell m}(r\Omega)\, \psi_{n'\ell'm'}(r\Omega) = \delta_{nn'}\delta_{\ell\ell'}\delta_{mm'}$$

$n = n_r + \ell + 1 \quad , \quad n_r = 0, 1, 2, \ldots \qquad (n_r = n - \ell - 1)$

$\ell = 0, 1, 2, \ldots, n-1$

$-\ell \leq m \leq \ell$

Laguerre

$$L_n^\alpha(x) = e^x \frac{x^{-\alpha}}{n!} d_x^n \left(e^{-x} x^{n+\alpha} \right), \quad n = 0, 1, 2, \cdots$$

$$L_n^\alpha(x) = \sum_{k=0}^{n} \frac{\Gamma(n+\alpha+1)}{\Gamma(k+\alpha+1)} \frac{(-x)^k}{k!\,(n-k)!}$$

$$(1-t)^{-\alpha-1} e^{-\frac{xt}{(1-t)}} = \sum_{n=0}^{\infty} L_n^\alpha(x)\, t^n$$

$$L_n^\alpha(x) = \frac{e^x x^{-\frac{\alpha}{2}}}{n!} \int_0^\infty t^{n+\frac{\alpha}{2}} J_\alpha(2\sqrt{xt})\, e^{-t}\, dt$$

$$L_n^\alpha(x) \xrightarrow[n\to\infty]{} \frac{e^{x/2}}{\sqrt{\pi}} n^{\frac{\alpha}{2}-\frac{1}{4}} x^{-\frac{\alpha}{2}-\frac{1}{4}} \cos\left\{ 2\sqrt{nx} - \frac{\alpha\pi}{2} - \frac{\pi}{4} \right\}$$

skoðum aðeins róf

$n = 1 \rightarrow l = 0,\ m = 0$ einfalt grunnástand 1s

$Y_{00}(\Omega)$ kúlusamhverfa

$n = 2 \rightarrow l = 0,\ m = 0$, kúlusamhverfa 2s

$$l = 1 \begin{cases} m = -1 \\ m = 0 \\ m = +1 \end{cases}$$

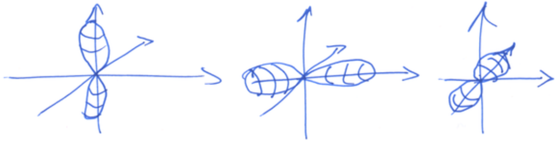
margföld

Ekki kúlusamhverf 2p

tölum of um px

py, pz

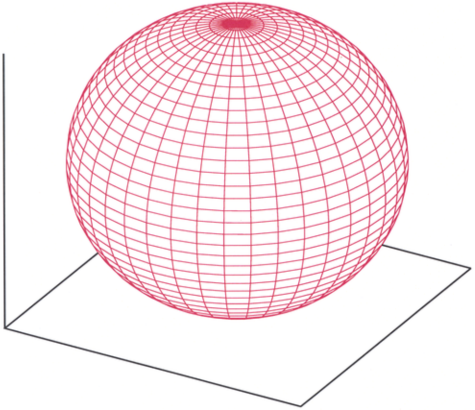
og teiknum of



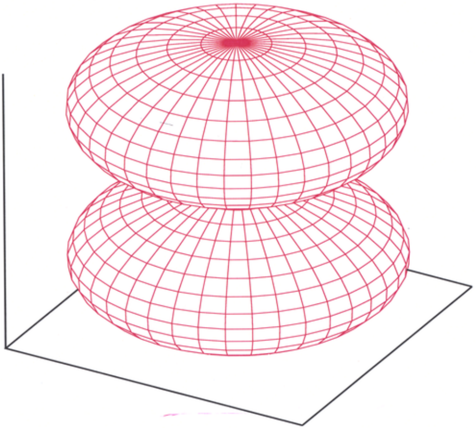
Eru þetta

$$|Y_{1,0\pm1}|^2 ?$$

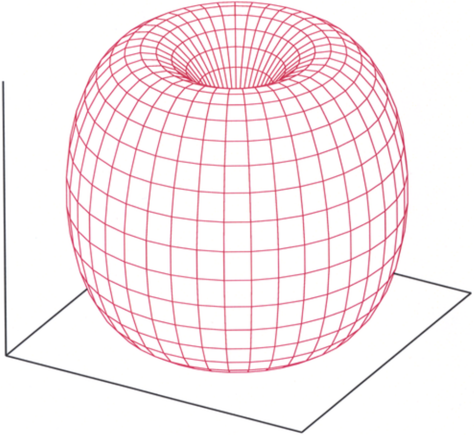
$|Y_{00}|^2$



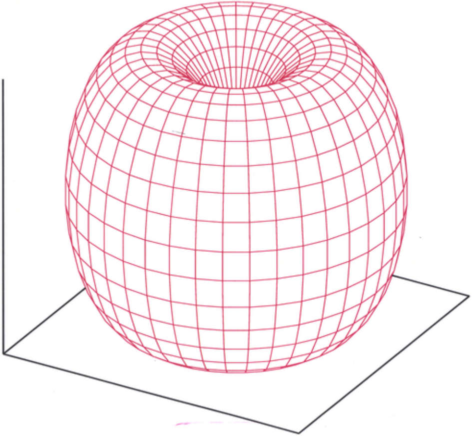
$|Y_{10}|^2$



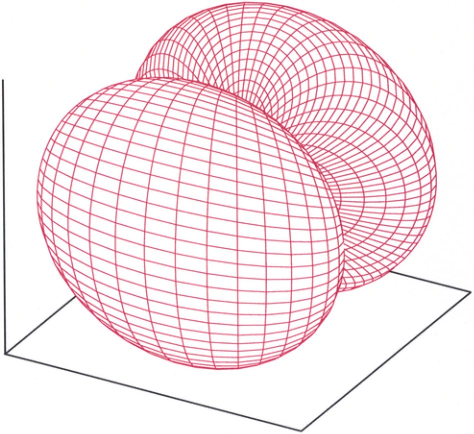
$|Y_{11}|^2$



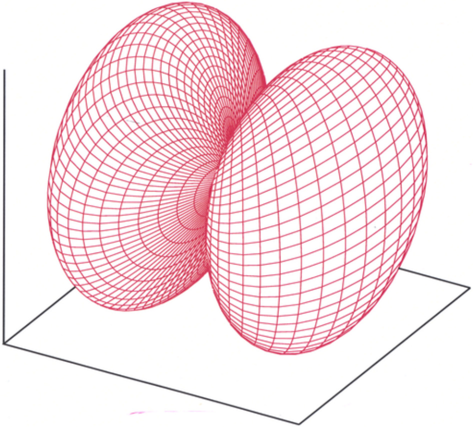
$|Y_{1-1}|^2$



$|Y_{11}+Y_{1-1}|^2$



$|Y_{11}-Y_{1-1}|^2$



margföld ástönd, 2p-ástönd

Eiginföllin $Y_{1,1}$, Y_{10} og $Y_{1,-1}$ spanna hlutrúmið en það gera líka

$$Y_{10} \quad \text{og} \quad \frac{1}{\sqrt{2}}\left[Y_{1,1} \pm Y_{1,-1} \right]$$

þau eru notuð í bókum til að tákna px, py, pz

Athyglisvert er líka

$$\sum_{m=-l}^{l} |Y_{lm}(\theta,\phi)|^2 = \frac{2l+1}{4\pi} \qquad \text{Kúlusamhverf}$$

Eftir það kanna betur hvert tilfinnga næsta verkefni

skoðum við síðar fínuppbyggingu vetnis

Er litrófið okkar of einfalt?

Truflanareikn

línuróf H er stýrt með jöfnu $E_\gamma = E_i - E_f = -R_y\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$

En ~~þessi~~ jafna er bara nálgun, hér þarf meira en einfaldan truflanareikning

↳ Dofnun, línubreidd, hnik og meðal orki