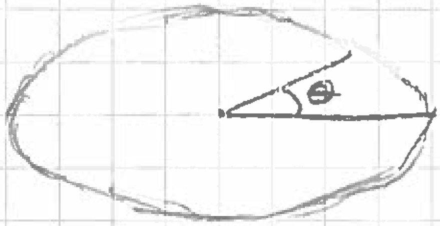
1

$$\frac{-\hbar^2}{2I}\frac{\partial^2\psi}{\partial\theta^2} = E\psi \qquad 0 \leq \theta < 2\pi$$



$$\psi = Ae^{im_\ell\theta} = Ae^{im_\ell(\theta+n2\pi)} = Ae^{im_\ell\theta}\underbrace{e^{in2\pi m_\ell}}_{=1}$$

jos n ja m_ℓ ovat kokonaislukuja

$$\frac{\partial^2\psi}{\partial\theta^2} = \frac{\partial}{\partial\theta}\left(A(im_\ell)\,e^{im_\ell\theta}\right)$$

$$= A(im_\ell)^2 e^{im_\ell\theta}$$

$$= -m_\ell^2 A e^{im_\ell\theta}$$

$$\frac{-\hbar^2}{2I}\frac{\partial^2\psi}{\partial\theta^2} = \frac{\hbar^2 m_\ell^2}{2I}Ae^{im_\ell\theta} = E\psi$$

$$E = \frac{\hbar^2 m_\ell^2}{2I}$$

$$N = \int_0^{2\pi}\psi^*\psi\,d\theta = \int_0^{2\pi}e^{-im_\ell\theta}e^{im_\ell\theta}\,dr = \int_0^{2\pi}1\,dr$$

$$= 2\pi$$

$$\Rightarrow \tilde{\psi} = \frac{1}{\sqrt{N}}\psi = \frac{1}{\sqrt{2\pi}}e^{im_\ell\theta}$$

2 a) $\hat{l}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$

$$= -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)$$

b) $\hat{l}_z = -i\hbar \frac{\partial}{\partial \phi}$

$$\psi_{m_l} = \cos(m_l \phi) + i \sin(m_l \phi) = e^{i m_l \phi}$$

$$\hat{l}_z \psi_{m_l} = -i\hbar \frac{\partial}{\partial \phi} e^{i m_l \phi} = \underbrace{\hbar m_l}_{l_z} \underbrace{e^{i m_l \phi}}_{\psi_{m_l}}$$

c) $\rho(\phi) = \frac{\psi^* \psi}{\langle \psi | \psi \rangle} = \frac{e^{-i m_l \phi} e^{i m_l \phi}}{\int_0^{2\pi} 1 \, \phi} = \frac{1}{2\pi}$

hiukkanen on yhtä todennäköisesti kaikkialla, kvanttiluku m_l kertoo kuinka nopeasti hiukkanen pyörii

③ $$\hat{l} = \hat{r}\times\hat{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = (yp_z - zp_y)\hat{i} + (zp_x - xp_z)\hat{j} + (xp_y - yp_x)\hat{k} = l_x\hat{i} + l_y\hat{j} + l_z\hat{k}$$

$$[\hat{l}_x, \hat{l}_y]\psi = \hat{l}_x\hat{l}_y\psi - \hat{l}_y\hat{l}_x\psi$$

$$\hat{l}_x\hat{l}_y\psi = (yp_z - zp_y)(zp_x - xp_z)\psi$$

järjestystä ei saa vaihtaa $\qquad$ saa vaihtaa

$$= (yp_z zp_x - yp_z xp_z - zp_y zp_x + \overbrace{zp_y}\, xp_z)\psi$$

$$= (p_z z\, yp_x - yx\, p_z^2 - z^2 p_y p_x + zp_z\, xp_y)\psi$$

$$\hat{l}_y\hat{l}_x\psi = (zp_x - xp_z)(yp_z - zp_y)\psi$$

$$= (zp_x yp_z - zp_x zp_y - xp_z yp_z + xp_z zp_y)\psi$$

$$= (zp_z\, yp_x - z^2 p_x p_y - xy\, p_z^2 + p_z z\, xp_y)\psi$$

$$(\hat{l}_x\hat{l}_y - \hat{l}_y\hat{l}_x)\psi =$$

$$\Big[p_z z\, yp_x - \cancel{yx\, p_z^2} - \cancel{z^2 p_y p_x} + zp_z\, xp_y$$

$$- (zp_z\, yp_x - \cancel{z^2 p_x p_y} - \cancel{xy\, p_z^2} + p_z z\, xp_y)\Big]\psi =$$

$$\Big[(p_z z - zp_z)\, yp_x + \underbrace{(zp_z - p_z z)}_{[\hat{z}, \hat{p}_z] = i\hbar} xp_y\Big]\psi =$$

$$-i\hbar\, yp_x + i\hbar\, xp_y =$$

$$i\hbar\, \hat{l}_z$$

$$[\hat{l}_x, \hat{l}_y] = i\hbar\, \hat{l}_z$$

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \rightarrow \begin{vmatrix} \hat{k} & \hat{i} & \hat{j} \\ z & x & y \\ p_z & p_x & p_y \end{vmatrix} \Rightarrow [\hat{l}_z, \hat{l}_x] = i\hbar\, l_y$$

(4) $R_{1,0} = 2\left(\frac{Z}{a}\right)^{3/2} e^{-\rho_1/2}$

$R_{2,0} = \frac{1}{8^{1/2}}\left(\frac{Z}{a}\right)^{3/2}(2-\rho_2)e^{-\rho_2/2}$

kulmaosa $Y_{0,0} = 1$ $\qquad \rho_n = \frac{2Zr}{n a_0}$

$$\langle \Psi_{1s} | \Psi_{2s} \rangle = 4\pi \int_0^\infty 2\left(\frac{Z}{a}\right)^{3/2} e^{-\rho_1/2} \frac{1}{8^{1/2}}\left(\frac{Z}{a}\right)^{3/2}(2-\rho)e^{-\rho_2/2} r^2 dr$$

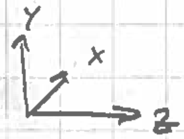
$$= 4\pi \frac{2}{8^{1/2}}\left(\frac{Z}{a}\right)^3 \int_0^\infty (2-\rho_2)\, e^{-\rho_1/2} e^{-\rho_2/2} r^2 dr$$

$$= \frac{8\pi}{\sqrt{8}}\left(\frac{Z}{a}\right)^3 \int_0^\infty \left(2 - \frac{1}{2}\rho_1\right) e^{-\rho_1/2} e^{-\frac{1}{2}\rho_1/2} \rho_1^2 \left(\frac{a_0}{2Z}\right)^2 d\rho_1$$

$$= \frac{\pi}{\sqrt{8}}\left(\frac{Z}{a}\right)^3 \left(\frac{a_0}{2Z}\right)^2 \int_0^\infty \left(2\rho_1^2 - \frac{1}{2}\rho_1^3\right) e^{-\frac{3}{4}\rho_1} d\rho_1$$

$$= \frac{\pi}{\sqrt{8}}\left(\frac{Z}{a}\right)^3\left(\frac{a}{2Z}\right)^2 \left[\underbrace{2\frac{2!}{(3/4)^3} - \frac{1}{2}\frac{3!}{(3/4)^4}}_{\frac{4}{(3/4)^3} - \underbrace{\frac{1}{\cancel{2}}\frac{4}{\cancel{3}}\frac{2\cdot\cancel{3}}{(3/4)^3}}_{4/(3/4)^3} = 0}\right]$$

$$= 0$$

(5) $2p_z$ orbitaali  

kulman ääriarvot ovat z-suuntaan

$$\psi_{2z} = R_{2,1}\, Y_{1,0}$$

todnäk. tiheys

$$\rho_{2p_z} = \psi_{2z}^* \psi_{2z} = |R_{2,1}|^2 |Y_{1,0}|^2$$

$$\nabla \rho_{2p_z} = \vec{0}$$

$$R_{2,1} = \frac{1}{\sqrt{24}} \left(\frac{Z}{a}\right)^{3/2} \rho_2 e^{-\rho_2/2}$$

$$\nabla \rho_{2z} = \left(\hat{r}\frac{\partial}{\partial r} + r^{-1}\hat{\phi}\frac{\partial}{\partial \phi} + r^{-1}\sin\phi\, \hat{\theta}\frac{\partial}{\partial \theta}\right)\rho_{2p_z}$$

$$= \left(\hat{r}\frac{\partial}{\partial r}|R_{2,1}|^2\right)|Y_{1,0}|^2 + \underbrace{r^{-1}|R_{2,1}|^2 \hat{\phi}\frac{\partial}{\partial \phi}|Y_{1,0}|^2 + r^{-1}\sin\phi\, |R_{2,1}|^2 \hat{\theta}\frac{\partial}{\partial \theta}|Y_{1,0}|^2}_{\text{kulmaosa} \;\to\; z \text{ suunta}}$$

$$\frac{\partial}{\partial r}|R_{2,1}|^2 = \frac{\partial}{\partial r}\left(\frac{1}{24}\left(\frac{Z}{a}\right)^3 \rho_2^2 e^{-\rho_2}\right)$$

$$= \frac{1}{24}\left(\frac{Z}{a}\right)^3 \frac{\partial}{\partial r}\left[\left(\frac{2Z}{2a}\right)^2 r^2 e^{-\frac{2Z}{2a}r}\right]$$

$$= \frac{1}{24}\left(\frac{Z}{a}\right)^3 \left(\frac{Z}{a}\right)^2 \left[2r e^{-Zr/a} - \frac{Zr^2}{a} e^{-Zr/a}\right]$$

$$\frac{\partial}{\partial r}(R_{2,1})^2 = 0 \implies \left(2r - \frac{Zr^2}{a}\right)e^{-Zr/a} = 0$$

$$\implies 2 - \frac{Zr}{a} = 0 \implies r = \frac{2a}{Z}$$

Todennäköisimmät kohdat $(0,0,2a_0)$ & $(0,0,-2a_0)$