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(1) $N \equiv N$

voimavakio $k = 2293{,}8 \frac{N}{m}$

$m_{^{14}N} = 14{,}0031\ u$

Redusoitu massa $\mu = \frac{m_{^{14}N} \cdot m_{^{14}N}}{m_{^{14}N} + m_{^{14}N}} = \frac{1}{2} m_{^{14}N}$

$= \frac{1}{2} \cdot 14{,}0031\ u \cdot 1{,}6605402 \cdot 10^{-27}\ kg/u$

$= 1{,}1626 \cdot 10^{-26}\ kg$

Nollapiste-energia: $E_0 = (0 + \frac{1}{2})\hbar\omega = \frac{1}{2}\hbar\omega$

$= \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}$

$= \frac{1}{2} \cdot 1{,}054573 \cdot 10^{-34}\ Js \cdot \sqrt{\frac{2293{,}8\ N/m}{1{,}1626 \cdot 10^{-26}\ kg}}$

$\approx 2{,}34 \cdot 10^{-20}\ J = 0{,}15\ eV$

②

harmoninen värähtelijä, $E = (\nu + \frac{1}{2})\hbar\omega$.

$$\psi_\nu(x) = \underset{\text{normitus-vakio}}{N_\nu} \underbrace{H_\nu(y)}_{\text{Hermiten polynomi}} e^{-y^2/2}, \quad y = \frac{x}{\alpha}, \quad \alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}, \quad N_\nu = \frac{1}{\sqrt{\alpha \pi^{1/2} 2^\nu \nu!}}$$

Tapaus $\langle x \rangle$ kirjassa esimerkki 9.4:

$$\underline{\underline{\langle x \rangle}} = \int_{-\infty}^{\infty} \psi_\nu^* \, x \, \psi_\nu \, dx = N_\nu^2 \int_{-\infty}^{\infty} (H_\nu e^{-y^2/2}) x (H_\nu e^{-y^2/2}) dx$$

$$= \alpha^2 N_\nu^2 \int_{-\infty}^{\infty} (H_\nu e^{-y^2/2}) y (H_\nu e^{-y^2/2}) dy$$

$$\left(\begin{array}{l} x = \alpha y, \\ \Rightarrow \frac{dx}{dy} = \alpha \\ \Rightarrow dx = \alpha dy \end{array} \right)$$

rekursio: $y H_\nu = \nu H_{\nu-1} + \frac{1}{2} H_{\nu+1}$

$$= \alpha^2 N_\nu^2 \int_{-\infty}^{\infty} H_\nu \, y H_\nu \, e^{-y^2} dy = \alpha^2 N_\nu^2 \int_{-\infty}^{\infty} H_\nu (\nu H_{\nu-1} + \tfrac{1}{2} H_{\nu+1}) e^{-y^2} dy$$

$$= \alpha^2 N_\nu^2 \Big[\underbrace{\nu \int_{-\infty}^{\infty} H_\nu H_{\nu-1} e^{-y^2} dy}_{=0} + \underbrace{\frac{1}{2} \int_{-\infty}^{\infty} H_{\nu+1} H_\nu e^{-y^2} dy}_{=0} \Big] = \underline{\underline{0}}$$

(*)

$$(*) \int_{-\infty}^{\infty} H_{\nu'} H_\nu e^{-y^2} dy = \begin{cases} 0, & \text{jos } \nu' \neq \nu \\ \pi^{1/2} 2^\nu \nu!, & \text{jos } \nu' = \nu \end{cases}$$

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② jatkuu

$$\underline{\underline{\langle x^2\rangle}} = \int_{-\infty}^{\infty} \psi_\nu^* x^2 \psi_\nu \, dx \underset{\substack{x=\alpha y \\ dx=\alpha dy}}{=} N_\nu^2 \int_{-\infty}^{\infty} y^2 \alpha^3 H_\nu^2(y)\, e^{-y^2} dy$$

$$= N_\nu^2 \alpha^3 \int_{-\infty}^{\infty} H_\nu y \cdot y H_\nu e^{-y^2} dy$$

rekursio-relaatio

$$= N_\nu^2 \alpha^3 \int_{-\infty}^{\infty} (\nu H_{\nu-1} + \tfrac{1}{2} H_{\nu+1})(\nu H_{\nu-1} + \tfrac{1}{2} H_{\nu+1}) e^{-y^2} dy$$

$$= N_\nu^2 \alpha^3 \int_{-\infty}^{\infty} (\nu^2 H_{\nu-1}^2 + \nu H_{\nu-1} H_{\nu+1} + \tfrac{1}{4} H_{\nu+1}^2) e^{-y^2} dy$$

$$= N_\nu^2 \alpha^3 \Big[\nu^2 \underbrace{\int_{-\infty}^{\infty} H_{\nu-1}^2 e^{-y^2} dy}_{=\pi^{1/2} 2^{\nu-1} (\nu-1)!} + \nu \underbrace{\int_{-\infty}^{\infty} H_{\nu-1} H_{\nu+1} e^{-y^2} dy}_{=0} + \tfrac{1}{4} \underbrace{\int_{-\infty}^{\infty} H_{\nu+1}^2 e^{-y^2} dy}_{=\pi^{1/2} 2^{\nu+1} (\nu+1)!}\Big]$$

$$= N_\nu^2 \alpha^3 \pi^{1/2} \left(\nu^2 2^{\nu-1} (\nu-1)! + \tfrac{1}{4} 2^{\nu+1} (\nu+1)!\right)$$

$$\left(N_\nu^2 = \frac{1}{\alpha \pi^{1/2} 2^\nu \nu!} = \frac{1}{\alpha \pi^{1/2} 2^\nu \nu (\nu-1)!} = \frac{(\nu+1)}{\alpha \pi^{1/2} 2^\nu (\nu+1)!} \right)$$

$$= \frac{\alpha^{\cancel{3}\,2} \cancel{\pi^{1/2}} \nu^{\cancel{2}} \cancel{2^{\nu-1}} \cancel{(\nu-1)!}}{\cancel{\alpha} \cancel{\pi^{1/2}} \underbrace{2^\nu}_{=2^{\nu-1}\cdot 2} \cancel{\nu} \cancel{(\nu-1)!}} + \frac{\alpha^{\cancel{3}\,2} \cancel{\pi^{1/2}} \overbrace{2^{\nu+1}}^{=2^\nu \cdot 2} \cancel{(\nu+1)!} (\nu+1)}{\cancel{4}_{2} \cancel{\alpha} \cancel{\pi^{1/2}} \cancel{2^\nu} \cancel{(\nu+1)!}}$$

$$= \frac{\alpha^2 \nu}{2} + \frac{\alpha^2 (\nu+1)}{2} = \frac{\alpha^2 \nu + \alpha^2 \nu + \alpha^2}{2}$$

$$= \alpha^2 \nu + \frac{\alpha^2}{2} = \alpha^2 (\nu + \tfrac{1}{2}) = \underline{\underline{(\nu + \tfrac{1}{2}) \cdot \frac{\hbar}{\sqrt{mk}}}}$$

$$\underline{\Delta x} = (\langle x^2\rangle - \langle x\rangle^2)^{1/2} = \left((\nu + \tfrac{1}{2}) \frac{\hbar}{\sqrt{\mu k}} - 0^2\right)^{1/2} = \left(\frac{\hbar}{2\sqrt{\mu k}}\right)^{1/2}$$

$$= \left(\frac{1{,}054573 \cdot 10^{-34}\,\mathrm{Js}}{2 \cdot \sqrt{1{,}1626 \cdot 10^{-26}\,\mathrm{kg} \cdot 2293{,}8\,\mathrm{N/m}}}\right)^{1/2} \approx \underline{\underline{3{,}20 \cdot 10^{-12}\,\mathrm{m}}}$$

(n. 3% N_2:n sidospituudesta 1,0975 Å)

③ (vrt. esimerkki 9.2. s.290 Atkinsin kirjassa)

Oletetaan tunneloitumisvirran olevan verrannollinen läpäisytodennäköisyyteen T.

Virta heikkenee, eli etäisyyttä kasvatetaan. Tällöin

$$\underset{\text{uusi etäisyys}}{T(L_2)} = 0{,}95\, \underset{\text{vanha etäisyys}}{T(L_1)}$$

eli läpäisytodennäköisyys pienenee 5 %.

$$\Rightarrow \frac{T(L_2)}{T(L_1)} = 0{,}95 \iff \frac{\cancel{16\varepsilon(1-\varepsilon)}e^{-2\kappa L_2}}{\cancel{16\varepsilon(1-\varepsilon)}e^{-2\kappa L_1}} = 0{,}95$$

$$\iff e^{-2\kappa(L_2-L_1)} = 0.95 \quad | \ln$$

$$\iff L_2 - L_1 = \frac{\ln 0.95}{-2\kappa} = \frac{\ln 0{,}95}{-2\left(\sqrt{\frac{2m_e(V-E)}{\hbar^2}}\right)}$$

$$= \frac{\ln 0.95}{-2\left(\sqrt{\frac{2\cdot 9{,}1094\cdot 10^{-31}\,\text{kg}\cdot(3\,\text{eV}\cdot 1{,}602\cdot 10^{-19}\,\text{J/eV})}{(1{,}0546\cdot 10^{-34}\,\text{Js})^2}}\right)}$$

$$= \frac{\ln 0{,}95}{-2\cdot 8{,}87287\cdot 10^{9}} \approx \underline{\underline{2{,}9\ \text{pm}}}$$

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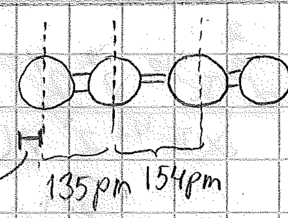
④ butadieeni $H_2C = CHCH = CH_2$

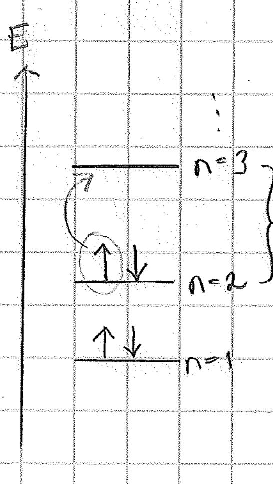
("hiukkanen laatikossa")



Hiilirungon pituus:

$$2\cdot 77\,\text{pm} + 2\cdot 135\,\text{pm} + 1\cdot 154\,\text{pm} = 578\,\text{pm} =: L$$

(1-dimensioisen laatikon koko)



Esim. Atkins, s. 281, kaava 9.7:

$$\Delta E = E_3 - E_2 = (2\cdot 2+1)\frac{h^2}{8mL^2}$$

$$= \frac{5\cdot(6{,}626\cdot 10^{-34}\,\text{Js})^2}{8\cdot 9{,}10939\cdot 10^{-31}\,\text{kg}\cdot(578\cdot 10^{-12}\,\text{m})^2}$$

$$\approx 9{,}0165\cdot 10^{-19}\,\text{J}$$

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④ jatkuu

$$\Delta E = h\nu \Rightarrow \nu = \frac{\Delta E}{h} = \ldots = 1{,}3608 \cdot 10^{15} \tfrac{1}{s}$$

$$\underline{\underline{\lambda}} = \frac{c}{\nu} = \frac{2{,}9979 \cdot 10^{8} \frac{m}{s}}{1{,}3608 \cdot 10^{15} \frac{1}{s}} = 2{,}203 \cdot 10^{-7} m \approx \underline{\underline{220\ nm}}$$

(vrt. kokeellinen arvo $\lambda = 217\ nm$)

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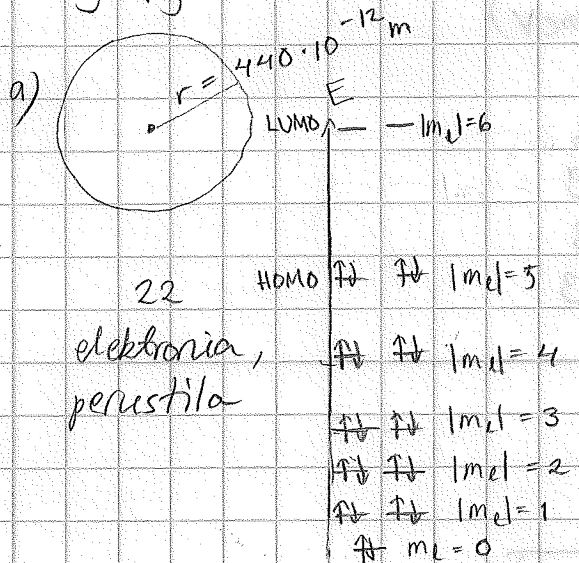
⑤ Porfyriini

Käsitellään π-elektronipilven elektronia "hiukkanen ympyräradalla" -tulosten avulla.

a)



$$\left\{ \begin{array}{l} l_z = m_l \hbar \\ E_{m_l} = \dfrac{m_l^2 \hbar^2}{2I} \\ (I = m_e r^2) \end{array} \right. \qquad m_l = 0, \pm 1, \pm 2, \ldots$$

b) $\underline{\underline{l_z}} = \pm 5\hbar = \pm 5 \cdot (1{,}0546 \cdot 10^{-34} Js) = \underline{\underline{\pm 5{,}27 \cdot 10^{-34} Js}}$

$$\underline{\underline{E_{\pm 5}}} = \frac{25 \cdot (1{,}0546 \cdot 10^{-34} Js)^2}{2 \cdot 9{,}109 \cdot 10^{-31} kg \cdot (440 \cdot 10^{-12} m)^2}$$

$$\approx \underline{\underline{7{,}88 \cdot 10^{-19} J}}$$

c) $\underline{\underline{l_z}} = \pm 6\hbar = \underline{\underline{\pm 6{,}33 \cdot 10^{-34} Js}}$ $\quad \underline{\underline{E_{\pm 6}}} = \ldots = \underline{\underline{1{,}14 \cdot 10^{-18} J}}$

$\Rightarrow \Delta E = 3{,}47 \cdot 10^{-19} J \qquad \Delta E = h\nu = \frac{hc}{\lambda}$

$$\Rightarrow \underline{\underline{\lambda}} = \frac{hc}{\Delta E} = \frac{6{,}626 \cdot 10^{-34} Js \cdot 2{,}9979 \cdot 10^{8} \frac{m}{s}}{3{,}47 \cdot 10^{-19} J} \approx \underline{\underline{570\ nm}}$$

(näkyvää valoa)

(6) ${}^{1}H^{127}I$

$$E = \frac{l(l+1)\hbar^2}{2I} = \frac{l(l+1)\hbar^2}{2\mu R^2}$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$= \frac{l(l+1)\hbar^2}{2R^2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

$$= l(l+1)\cdot \frac{(1{,}0546\cdot 10^{-34}\,Js)^2}{2\cdot(160\cdot 10^{-12}\,m)^2}\cdot\left(\frac{1}{1{,}008} + \frac{1}{126{,}90}\right)\underbrace{\frac{1}{1{,}6605\cdot 10^{-27}\,kg}}_{=u}$$

$$= l(l+1)\cdot 1{,}308\cdot 10^{-22}\,J$$

l	E $(\cdot 10^{-22}\,J)$	E (meV)
0	0	0
1	2,62	1,6
2	7,85	4,9
3	15,70	9,8
4	26,16	16,3

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(7) $V = 1{,}5\,eV$
$L = 1\,nm$

a) $E = 1\,eV$ $\qquad KL = \sqrt{\frac{2m_e(V-E)}{\hbar^2}}\,L$

$$= 1\cdot 10^{-9}\,m\sqrt{\frac{2\cdot 9{,}1094\cdot 10^{-31}\,kg\cdot(1{,}5eV - 1eV)\cdot 1{,}602\cdot 10^{-19}\,J/eV}{(1{,}054573\cdot 10^{-34}\,Js)^2}}$$

$$= 3{,}6224 > 1 \Rightarrow T \approx 16\cdot\left(\frac{E}{V}\right)\left(1-\left(\frac{E}{V}\right)\right)e^{-2KL}$$

$$= 16\cdot\left(\frac{1\,eV}{1{,}5\,eV}\right)\left(1 - \frac{1eV}{1{,}5eV}\right)e^{-2\cdot 3{,}6224} \approx \underline{\underline{0{,}0025}}$$

b) $E = 0{,}01eV \Rightarrow kL = 6{,}2533 > 1$

$$\Rightarrow T \approx 16\cdot\left(\frac{0{,}01eV}{1{,}5eV}\right)\left(1 - \frac{0{,}01eV}{1{,}5eV}\right)e^{-2\cdot 6{,}2533} \approx \underline{\underline{3{,}9\cdot 10^{-7}}}$$

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(8) $\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$ $\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$

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

$\underline{\underline{[\hat{L}_x, \hat{L}_y]}}\psi = \left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right)\psi$

$= -\hbar^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]\psi$

$= -\hbar^2\left[\underbrace{y\frac{\partial}{\partial z}z\frac{\partial}{\partial x}}_{= y\left(\frac{\partial}{\partial x} + z\frac{\partial^2}{\partial z\partial x}\right)} - y\frac{\partial}{\partial z}x\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}z\frac{\partial}{\partial x} + z\frac{\partial}{\partial y}x\frac{\partial}{\partial z}\right.$

$\left. - z\frac{\partial}{\partial x}y\frac{\partial}{\partial z} + z\frac{\partial}{\partial x}z\frac{\partial}{\partial y} + x\frac{\partial}{\partial z}y\frac{\partial}{\partial z} - \underbrace{x\frac{\partial}{\partial z}z\frac{\partial}{\partial y}}_{= x\left(\frac{\partial}{\partial y} + z\frac{\partial^2}{\partial z\partial y}\right)}\right]\psi$

tulon derivoimissääntö

$= -\hbar^2\left[y\frac{\partial}{\partial x} + \cancel{yz\frac{\partial^2}{\partial z\partial x}} - \cancel{xy\frac{\partial^2}{\partial z^2}} - \cancel{z^2\frac{\partial}{\partial y\partial x}} + \cancel{zx\frac{\partial^2}{\partial y\partial z}}\right.$

$\left. - \cancel{zy\frac{\partial^2}{\partial x\partial z}} + \cancel{z^2\frac{\partial^2}{\partial x\partial y}} + \cancel{xy\frac{\partial^2}{\partial z^2}} - x\frac{\partial}{\partial y} - \cancel{xz\frac{\partial^2}{\partial z\partial y}}\right]\psi$

$= -\hbar^2\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\psi = \frac{-\hbar^2}{i\hbar}\hat{L}_z\psi = -\frac{\hbar}{i}\hat{L}_z\psi = \underline{\underline{i\hbar\hat{L}_z}}\psi$

↑
derivoimisjärjestystä saa vaihtaa (aaltofunktiot siististi käyttäytyviä)

Emme voi määrittää tarkasti kuin yhden pyörimismääräkomponentin kerrallaan.