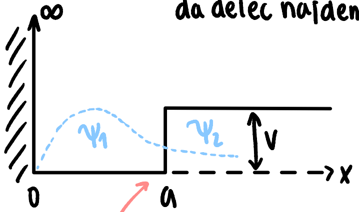
39.naloga – Potencialna jama (1D), v njej delec, ki ga opisuje Ψ_1. Kolikšna je verjetnost, da delec najdemo zunaj jame?



$\Psi_1 = A\cdot \sin kx$
$ka = 2\pi/3$
$E = 3/4\, V$

$$P(\text{zunaj}) = \int_a^{\infty} |\Psi_2|^2 dx$$

$$P(V) = \int_V |\Psi|^2 dV$$

Tu se Ψ_1 in Ψ_2 zlepita, zato: $\Psi_1(a) = \Psi_2(a)$, $\Psi_1'(a) = \Psi_2'(a)$

$k = \sqrt{2mE}/\hbar$
$K = \sqrt{2m(V-E)}/\hbar$

Ker gre $\Psi_2 \to \infty$ je edina možnost: $\Psi_2 = B\cdot e^{-Kx}$

$A\cdot \sin ka = B\cdot e^{-Ka}$ oz $B = Ae^{Ka}\cdot \sin ka$

vst.

$$k\cdot \cancel{A}\cos ka = \cancel{A}\cancel{e^{Ka}}\cdot \sin ka\cdot(-K)\cdot \cancel{e^{-Ka}}$$

$$\boxed{\underbrace{\operatorname{tg} ka}_{\text{To poznamo}} = -\frac{k}{K}} \rightarrow \operatorname{tg}\frac{2\pi}{3} = \operatorname{tg} 120^\circ = -\sqrt{3} \Rightarrow k = \sqrt{3}\cdot K \Rightarrow Ka = ka/\sqrt{3} = \frac{2\pi}{3\sqrt{3}}$$

Izračunajmo še A:
$$P = \underbrace{\int_0^a |\Psi_1|^2 dx}_{I_1} + \underbrace{\int_a^{\infty} |\Psi_2|^2 dx}_{I_2} = 1$$

$$I_1 = A^2 \int_0^a \sin^2 kx\, dx = A^2 \int_0^a \frac{1-\cos 2kx}{2} dx = \frac{A^2}{2}\left(a - \frac{\sin 2ka}{k}\right)$$

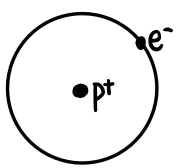
$$I_2 = A^2 e^{2Ka} \sin^2 ka \underbrace{\int_a^{\infty} e^{-2Kx} dx}_{\left.\frac{e^{-2Kx}}{-2K}\right|_a^{\infty}} = A^2 \cancel{e^{2Ka}}\cdot \sin^2 ka \cdot \frac{\cancel{e^{-2Ka}}}{2K}$$

$$P(\text{zunaj}) = \frac{I_2}{I_1+I_2} = \frac{1}{1+I_1/I_2}$$

$$\frac{I_1}{I_2} = \frac{a - \frac{\sin 2ka}{k}}{\sin^2 ka/K} = \frac{Ka - a\cdot \frac{\sin^2 ka}{ka}}{\sin^2 ka}$$

$\Rightarrow T = 0{,}34$

ATOM VODIKA



$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} - \frac{\alpha\hbar c}{r} \; ; \; \alpha = \frac{1}{137} = \frac{e^2}{4\pi\varepsilon_0\hbar c}$$

$r^2 = x^2 + y^2 + z^2$

$$\Psi = R_{nl}(r)\cdot \underbrace{Y_{lm}(\theta,\varphi)}_{\text{sferični harmoniki}}$$

$n = 1, 2, \ldots$
$l = 0, \ldots, n-1$
$m = -l, -l+1, \ldots, l-1, l$

$2l+1$ ... št. stanj z istim l $\Rightarrow$ degeneracija

$$\hat{H}\Psi_{nlm} = E_n \Psi_{nlm}$$

$$E_n = -\frac{\alpha^2 mc^2}{2}\cdot\frac{1}{n^2} \; ; \; E_1 = -13{,}6\,\text{eV}$$

$$\int \Psi^*_{n'l'm'} \Psi_{nlm} \underbrace{dV}_{r^2 dr\, d\cos\theta\, d\varphi} = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$

$$\Rightarrow \int_{-1}^{1}\int_0^{2\pi} Y^*_{l'm'} Y_{lm}\, d\cos\theta\, d\varphi = \delta_{ll'}\delta_{mm'} \; ; \; \int_0^{\infty} R^*_{n'l'} R_{nl}\, r^2 dr = \delta_{nn'}$$

Sferični harmoniki

$$Y_{\ell m}(\theta,\varphi)=(-1)^m\sqrt{\frac{2\ell+1}{4\pi}\cdot\frac{(\ell-m)!}{(\ell+m)!}}\,P_{\ell m}(\cos\theta)\cdot e^{im\varphi}$$

$\ell=0: m=0 \quad Y_{00}=\frac{1}{\sqrt{4\pi}}$

$\ell=1: m=\pm1 \quad Y_{1\pm1}=\mp\sqrt{3/8\pi}\cdot\sin\theta\cdot e^{\pm i\varphi}$

$\quad m=0 \quad Y_{10}=\sqrt{3/4\pi}\cdot\cos\theta$

$\ell=2: m=0 \quad Y_{20}=\sqrt{5/8\pi}\,(3\cos^2\theta-1)$

$\quad m=\pm1 \quad Y_{2\pm1}=\mp\sqrt{15/8\pi}\cdot(\sin\theta\cos\theta)e^{\pm i\varphi}$

$\quad m=\pm2 \quad Y_{2\pm2}=\sqrt{15/32\pi}\cdot\sin^2\theta\cdot e^{\pm2i\varphi}$

Kvantna meh.

$\vec{L}=\vec{r}\times\vec{p} \longrightarrow \hat{L}^2,\ \hat{L}_x,\hat{L}_y,\hat{L}_z$

Sferični harmoniki so lastna stanja za

$\hat{L}^2 Y_{\ell m}=\hbar^2\ell(\ell+1)Y_{\ell m}$

$\hat{L}_z Y_{\ell m}=\hbar m\cdot Y_{\ell m}$

$\vec{L}=\vec{r}\times(-i\hbar\vec{\nabla})$ kartezične koord.

$\hat{L}_z=-i\hbar\frac{d}{d\varphi}$

54. naloga – Atom vodika v stanju, ki ga opišemo s Ψ, zanima nas $\langle L_z\rangle$, če velja

$$\int f(r,\vartheta)\cdot f^*(r,\vartheta)\,r^2dr\,d\cos\vartheta=1$$

$$\Psi=\frac{1}{2\sqrt{\pi}}f(r,\vartheta)\cdot\cos(\varphi+i\sqrt{3}\cdot\sin\varphi)$$

$$\langle L_z\rangle=\int_V\Psi^*\hat{L}_z\Psi\,dV=\frac{1}{4\pi}\underbrace{\int f^2r^2dr\,d\cos\vartheta}_{1}\cdot\int_0^{2\pi}\underbrace{(\cos\varphi-i\sqrt{3}\cdot\sin\varphi)}_{\Psi^*}\cdot\underbrace{(-i\hbar)}_{iz\ \hat{L}_z}\underbrace{(-\sin\varphi+i\sqrt{3}\cdot\cos\varphi)}_{d\Psi/d\varphi}d\varphi$$

$$\langle L_z\rangle=-\frac{i\hbar}{4\pi}\int_0^{2\pi}i\sqrt{3}(\cos^2\varphi+\sin^2\varphi)+\underbrace{\cos\varphi\sin\varphi(-1+3)}_{=\sin(2\varphi)}=\frac{\sqrt{3}\hbar}{4\pi}\cdot2\pi=\frac{\hbar}{2}\cdot\sqrt{3}$$

$$\int_0^{2\pi}\sin(2\varphi)d\varphi=0$$

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$$\Psi=\frac{1}{\sqrt{2}}(Y_{10}+Y_{11})=\sqrt{\frac{3}{8\pi}}\left(\cos\theta-\frac{1}{\sqrt{2}}\cdot\sin\theta\,e^{i\varphi}\right)$$

$\langle L_x\rangle,\langle L_y\rangle,\langle L_z\rangle=?$

$$\hat{L}_x=i\hbar\left(\underset{\sin\varphi}{s_\varphi}\frac{d}{d\theta}+\frac{c_\varphi}{t_\theta}\frac{d}{d\varphi}\right)\ ;\ \langle L_x\rangle=\int_{-1}^{1}\int_0^{2\pi}\Psi^*L_x\Psi\,d\cos\theta\,d\varphi$$

$$\langle L_x\rangle=\frac{3}{8\pi}\int\left(c_\theta-\frac{1}{\sqrt{2}}s_\theta e^{-i\varphi}\right)\left(\frac{e^{i\varphi}-e^{-i\varphi}}{2i}\left(-\sin\theta-\frac{1}{\sqrt{2}}\cos\theta e^{i\varphi}\right)+\frac{e^{i\varphi}+e^{-i\varphi}c_\theta}{2\cdot s_\theta}\left(-\frac{i}{\sqrt{2}}s_\theta\cdot e^{i\varphi}\right)\right)$$

Upoštevamo $\int_0^{2\pi}e^{\pm i\varphi}d\varphi=0$ in $\int_0^{2\pi}d\varphi=2\pi$

$$\Rightarrow\langle L_x\rangle=\frac{3}{8\pi}\int_{-1}^{1}dc_\theta\left(-\frac{ic_\theta^2}{2\sqrt{2}}+\frac{s_\theta^2}{2\sqrt{2}\cdot i}+\frac{c_\theta^2}{2\sqrt{2}\cdot i}\right)\cdot2\pi=\frac{3\hbar}{4\cdot2\sqrt{2}}\cdot\int_{-1}^{1}(1+c_\theta^2)dc_\theta=\frac{\cancel{8}}{\cancel{3}}\cdot\frac{\cancel{3}\hbar}{\cancel{4\cdot2}\sqrt{2}}=\frac{\hbar}{\sqrt{2}}$$

Kaj delamo?

$$\langle L_y\rangle = \frac{3i\hbar}{8\pi}\int_0^{2\pi} d\varphi \int_{-1}^{1} dc_\theta \underbrace{\left(c_\theta - \frac{1}{\sqrt{2}} s_\theta e^{i\varphi}\right)}^{\psi^*}\left(-\frac{e^{i\varphi}+e^{-i\varphi}}{2}\cdot\left(-s_\theta - \frac{1}{\sqrt{2}}\cdot s_\theta e^{i\varphi}\right) + \frac{e^{i\varphi}-e^{-i\varphi}}{2i}\cdot\frac{c_\theta}{\cancel{s_\theta}}\cdot\frac{-i}{\sqrt{2}}\cdot\cancel{s_\theta} e^{i\varphi}\right) =$$

$$= \frac{3i\hbar}{8\pi}\cdot 2\pi\cdot\int_{-1}^{1} dc_\theta\left(\frac{1}{2\sqrt{2}}2\cdot c_\theta^2 - \frac{1}{2\sqrt{2}}\underbrace{s_\theta^2}_{1-c_\theta^2}\right) = \frac{3i\hbar}{8\sqrt{2}}\underbrace{\int_{-1}^{1} dc_\theta\left(2c_\theta^2 + c_\theta^2 - 1\right)}_{3\cdot\frac{c_\theta^3}{3}\Big|_{-1}^{1} - c_\theta\Big|_{-1}^{1} = 2-2=0} = 0$$

$$\langle L_z\rangle = -\frac{3i\hbar}{8\pi}\int_0^{2\pi} d\varphi\int_{-1}^{1} dc_\theta\left[c_\theta - \frac{1}{\sqrt{2}}\cdot s_\theta\cdot e^{-i\varphi}\right]\cdot\frac{-i}{\sqrt{2}}\cdot s_\theta e^{i\varphi} = -\frac{3\hbar}{8\pi}\cdot 2\pi\cdot\int_{-1}^{1} dc_\theta - \frac{1}{2}(1-c_\theta^2) = \frac{3\hbar}{8}\left(2-\frac{2}{3}\right) = \frac{\hbar}{2}$$

Namesto direktnega računanja uporabimo pravil za lastna stanja / zvezami med sferičnimi harmoniki:

Vemo: $\int_\Omega Y^*_{l'm'} Y_{lm} = \delta_{l'l}\delta_{m'm}$ ortonormiran set

$$\int_\Omega Y^*_{l'm'}\hat{L}_x Y_{lm} = \frac{\hbar}{2}\sqrt{l(l+1)-m(m\pm1)}\cdot\delta_{l'l}\cdot\delta_{m'm\pm1}$$

$$\int_\Omega Y^*_{l'm'}\hat{L}_y Y_{lm} = \mp\frac{i\hbar}{2}\sqrt{l(l+1)-m(m\pm1)}\,\delta_{l'l}\,\delta_{m'm\pm1}$$

$$\int_\Omega Y^*_{l'm'}\underbrace{\hat{L}_z Y_{lm}}_{\hbar m Y_{lm}} = \hbar m\,\delta_{l'l}\,\delta_{m'm}$$

$$\int_\Omega Y^*_{l'm'}\hat{L}^2 Y_{lm} = \hbar^2 l(l+1)\,\delta_{l'l}\,\delta_{m'm}$$

Zdaj lahko na še 1 način poračunamo našo valovno funkcijo $\psi = \frac{1}{\sqrt{2}}(Y_{10}+Y_{11})$

$$\langle L_x\rangle = \frac{1}{2}\int_\Omega (Y_{10}^* + Y_{11}^*)\hat{L}_x(Y_{10}+Y_{11}) = \frac{1}{2}\int_\Omega(Y_{10}^*\hat{L}_x Y_{11} + Y_{11}^*\hat{L}_x Y_{10}) = \frac{\hbar}{4}\left(\sqrt{1\cdot2-1(1-1)} + \sqrt{1\cdot2-0(0+1)}\right) = \frac{\hbar}{\cancel{4}_2}\cdot\cancel{2}\sqrt{2} = \frac{\hbar}{\sqrt{2}}$$

Neničelno bomo dobili le, če množimo to med sabo

$$\langle L_y\rangle = \frac{1}{2}\int(Y_{10}^* L_y Y_{11} + Y_{11}^* L_y Y_{10}) = \frac{i\hbar}{4}(+\sqrt{2}-\sqrt{2}) = 0$$

$$\langle L_z\rangle = \frac{1}{2}\int(Y_{10}^* L_z Y_{10} + Y_{11}^* L_z Y_{11}) = \frac{1}{2}(\hbar\cdot 0 + \hbar\cdot 1) = \frac{\hbar}{2}$$

$$\langle L^2\rangle = \frac{1}{2}\int Y_{10}^*\hat{L}^2 Y_{10} + Y_{11}^*\hat{L}^2 Y_{11} = \frac{\hbar^2}{2}(1\cdot(1+1) + 1\cdot(1+1)) = 2\hbar^2$$

55. naloga

Kolikšna je verjetnost, da naletimo v vodikovem atomu na elektron v osnovnem stanju zunaj krogle z radijem, ki je enak povprečni oddaljenosti elektrona od jedra?

Osn. stanje: $n=1, \ell=0, m=0$

$$\psi_{n\ell m} = R_{n\ell}(r)\,Y_{\ell m}(\theta,\varphi) \Rightarrow \psi_{100} = \frac{1}{\sqrt{4\pi}}\cdot\frac{2}{r_B^{3/2}}\cdot e^{-r/r_B} \; ; \; r_B = \frac{\hbar c}{\alpha m_e c^2}$$

$$\langle r\rangle = \int_V \psi^* r \psi \, dV = \qquad dV = r^2 dr \underbrace{dc_\theta \, d\varphi}_{4\pi}$$

$$= \int_0^\infty \frac{4}{r_B^3} e^{-\frac{2r}{r_B}} r \cdot r^2 dr \; ; \; \frac{2r}{r_B} = t, \; dr = \frac{r_B}{2}dt \qquad P(n+1) = \int_0^\infty t^n e^{-t} dt = n!$$

$$\langle r\rangle = \int_0^\infty \frac{4}{r_B^3}\cdot e^{-t}\left(\frac{r_B}{2}\right)^4 t^3 dt = \frac{r_B}{4}\int_0^\infty \underbrace{t^3 e^{-t} dt}_{3!} = \frac{3}{2} r_B$$

$$P(\in V) = \int_V |\psi|^2 dV$$

$x = t-3$, $dx = dt$

$$P(r>\langle r\rangle) = \int_{\langle r\rangle}^\infty |\psi|^2 dV = \int_{3/2 r_B}^\infty \frac{4}{r_B^3} e^{-\frac{2r}{r_B}} r^2 dr = \frac{4}{r_B^3}\int e^{-t}\left(\frac{r_B}{2}\right)^3 t^2 dt = \frac{1}{2}\int_3^\infty e^{-t} t^2 dt = \frac{1}{2}\int_0^\infty e^{-x} e^{-3}(x+3)^2 dx =$$

$$= \frac{e^{-3}}{2}\int_0^\infty \underbrace{(x^2+6x+9)e^{-x} dx}_{2!+6\cdot 1!+9\cdot 0!} = e^{-3}\cdot\frac{17}{2} \approx 0{,}42$$

57. naloga

Atom vodika v stanju s kvantnimi števili $n=2$, $l=1$ in $m_l=0$ opiše lastna valovna funkcija

$$\frac{1}{2\sqrt{8\pi r_B^3}}\frac{r}{r_B}\exp\left(\frac{-r}{2r_B}\right)\cos\vartheta\,.$$

Kolikšna je povprečna vrednost potencialne energije? Primerjaj rezultat z rezultatom, ki ga predvideva Bohrov račun za elektron v stanju z glavnim kvantnim številom 2.

a) $\langle V\rangle = ?$

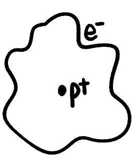
b) $\langle V\rangle_{Bohr} = ?$

$$\hat V = -\frac{\alpha\hbar c}{r} = -\alpha\hbar c\cdot\widehat{\left(\frac{1}{r}\right)}$$

$$\langle V\rangle = -\alpha\hbar c\int_0^\infty\int_{-1}^1 \frac{1}{32\pi r_B^3}\left(\frac{r}{r_B}\right)^2 e^{-\frac{r}{r_B}} c_\theta^2 \frac{1}{r}\cdot\overbrace{2\pi\cdot dc_\theta\, r^2 dr}^{dV} = -\frac{\alpha\hbar c}{16 r_B^3}\cdot\int_{-1}^1 c_\theta^2\, dc_\theta \int_0^\infty \frac{r^3}{r_B^3} e^{-\frac{r}{r_B}}\frac{dr}{r_B} \; ; \; t = \frac{r}{r_B}$$

$$= -\frac{\alpha\hbar c}{16 r_B}\cdot\frac{2}{3}\cdot 3! = -\frac{\alpha\hbar c}{4 r_B} \; ; \; r_B = \frac{\hbar c}{mc^2\alpha} \Rightarrow \boxed{\langle V\rangle = -\frac{\alpha^2 mc^2}{4}}$$

b) Bohrov model atoma H:



$$\lambda_{DB} = \frac{h}{p}$$

$$2\pi r = n\cdot\lambda = \frac{nh}{p}$$

$$p = \frac{nh}{2\pi r} = \frac{n\hbar}{r}$$

$$F_c = F_e = \frac{\alpha\hbar c}{r^2}$$

$$F_c = \frac{mv^2}{r} = \frac{p^2}{mr}$$

$$\Rightarrow \frac{n^2\hbar^2 \cancel{c^2}}{m r^{\cancel{3}}} = \frac{\alpha\hbar \cancel{c}}{\cancel{r^2}} \Rightarrow \boxed{\text{Bohr: } r \approx n^2\frac{\hbar c}{mc^2\alpha} = n^2 r_B}$$