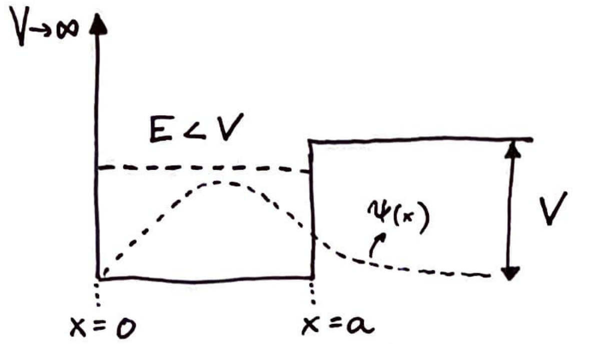
39 Pobeg iz pol-neskončne potencialne jame.



$E = 3/4\, V < V \,, \quad ka = \frac{2\pi}{3} = 120°,$

$\psi_1 = A \sin(kx) \,, \quad k = \frac{\sqrt{2mE}}{\hbar} ,$

$\psi_2 = B\, e^{-Kx} \,, \quad K = \frac{\sqrt{2m(V-E)}}{\hbar} .$

$\psi_1(0) = 0$ ok ✓ $\qquad \psi_1(a) = \psi_2(a),$

$A \sin(ka) = B e^{-Ka} \Rightarrow B = A \sin(ka)\, e^{Ka},$

$\psi_2(x) = A \sin(ka)\, e^{-K(x-a)},$

$\psi_1'(a) = \psi_2'(a),$

$\cancel{A}\, k \cos(ka) = \cancel{A} \sin(ka)(-K)\, e^{-K\overset{0}{(a-a)}},$

$\mathrm{tg}(ka) = -\frac{ka}{Ka} \Rightarrow \frac{1}{Ka} = -\frac{1}{ka}\mathrm{tg}(ka) = -\frac{3}{2\pi}\underbrace{\mathrm{tg}(120°)}_{-\sqrt{3}},$

$$\boxed{Ka = \frac{2\pi}{3\sqrt{3}}.}$$

1) Normalizacija : $1 = \overset{I_1}{\int_0^a |\psi_1|^2 dx} + \overset{I_2}{\int_a^\infty |\psi_2|^2 dx} \Rightarrow A$

2) Verjetnost da pobegne : I_2.

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

$I_2 = A^2 \sin^2(ka) \int_a^\infty e^{-2K(x-a)} dx = A^2 \sin^2(ka) \int_0^\infty \frac{1}{2K} e^{-t} dt = \frac{A^2}{2K}\sin^2(ka)$

$\left(-e^{-t}\Big|_0^\infty\right) = -e^{-\infty} - (-1) = 1$

$\Rightarrow A^2 \frac{a}{2}\left(1 - \frac{\sin 2ka}{2ka} + \frac{\sin^2 ka}{Ka}\right) = 1$

$$P(x>a) = I_2 = \frac{A^2 a}{2}\,\frac{\sin^2(ka)}{ka} = \frac{\sin^2(ka)}{Ka\left(1-\frac{\sin 2ka}{2ka}+\frac{\sin^2(ka)}{Ka}\right)}$$

$$= \frac{1}{1+\frac{Ka}{\sin^2(ka)}-\frac{Ka}{2ka}\,\frac{\sin(2ka)}{\sin^2(ka)}} = \underline{\underline{0{,}34.}}$$

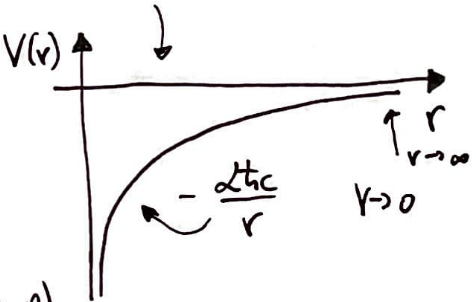
kjer smo uporabili : $Ka = \frac{2\pi}{3\sqrt{3}}$, $ka = \frac{2\pi}{3}$ in :

$$\sin(ka) = \sin\left(\frac{2\pi}{3}\right) = \frac{\sqrt{3}}{2},$$

$$\sin(2ka) = \sin\left(\frac{4\pi}{3}\right) = -\frac{\sqrt{3}}{2}.$$

Atom vodika in sferični harmoniki

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



Za poljuben sferično simetričen potencial velja: $\Psi = \psi_{nl}(r)\,Y_{lm}(\theta,\varphi)$

radialni del — sferični harmoniki

v 3D

$x = r\cos\theta\cos\varphi$

$y = r\cos\theta\sin\varphi$

$z = r\sin\theta$

$$\int dV = \int_0^{R\to\infty} r^2\,dr \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)$$

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

Lastne energije : $E_n = -\frac{mc^2}{2}\alpha^2\frac{1}{n^2}$, $n = 1, 2, \ldots$

$$= -E_{Ry}\frac{1}{n^2} \;,\quad E_{Ry} = -E_1 = 13{,}6\ \mathrm{keV}.$$

so negativne $\Rightarrow$ vezana stanja ; $n\to\infty$, $E_n \to 0$.

Lastne funkcije so ortonormirane po n, l in m:

$$\int \psi^*_{n'l'm'} \psi_{nlm} \, dV = \delta_{nn'} \delta_{ll'} \delta_{mm'}$$

$$dV = r^2 dr \, d\Omega \, , \quad d\Omega = d\varphi \, d(\cos\theta) \, .$$

Ortonormalnost je ločena po r in (θ, φ):

$$\psi_{nlm} = R_{nl}(r) \, Y_{lm}(\theta, \varphi) \quad \text{in:} \quad \int_0^\infty R_{n'l'} R_{nl} \, r^2 dr = \delta_{nn'} \, ,$$

$$\int_\Omega d\Omega \, Y^*_{l'm'} Y_{lm} = \delta_{ll'} \delta_{mm'} \, .$$

Radialni del je odvisen od $V(r)$, sferični del pa je univerzalen in ga bomo obravnavali za poljuben rotator.

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

$l = 0$, $m = 0$, $Y_{00} = \frac{1}{\sqrt{4\pi}}$,

$l = 1$, $m = 0, \pm 1$, $Y_{10} = \sqrt{\frac{3}{4\pi}} \underbrace{\cos\theta}_{c}$, $Y_{1\pm1} = \mp \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\varphi}$.

$l = 2$, $m = 0, \pm 1, \pm 2$, $Y_{20} = \sqrt{\frac{5}{8\pi}} (3c^2 - 1)$,

$$Y_{2\pm1} = \mp \sqrt{\frac{15}{8\pi}} \, c \sqrt{1-c^2} \, ,$$

$$Y_{2\pm2} = \sqrt{\frac{15}{32\pi}} (1-c^2) \, e^{\pm 2i\varphi} \, .$$

v splošnem je za vsak l na voljo $2l+1$ stanj.

$l = 3$, $m = 0, \pm 1, \pm 2, \pm 3$

$\vdots$

(54) Atom vodika : $\psi = \frac{1}{2\sqrt{\pi}} f(r,\theta) \left(\cos\varphi + i\sqrt{3}\sin\varphi\right)$

normaliziran

$L_z = -i\hbar \frac{d}{d\varphi}$ $\qquad$ $\int_0^\infty dr \int_{-1}^{1} d(\cos\theta)\, r^2 f(r,\theta)^2 = 1$

projekcija vrtilne količine na z-os.

$$\langle L_z \rangle = \int_V \psi^* \hat{L}_z \psi \, dV = \frac{1}{4\pi} \underbrace{\int_0^\infty \int_{-1}^{1} r^2 dr\, d(\cos\theta)\, f^2(r,\theta)}_{=1}$$

$$\times \int_0^{2\pi} d\varphi \left(c_\varphi - i\sqrt{3}s_\varphi\right)(-i\hbar)\left(-s_\varphi + i\sqrt{3}c_\varphi\right)$$

$$= -\frac{i\hbar}{4\pi} \int_0^{2\pi} d\varphi \left(i\sqrt{3}\underbrace{(s_\varphi^2 + c_\varphi^2)}_{1} \underbrace{- c_\varphi s_\varphi + 3 c_\varphi s_\varphi}\right)$$

$2c_\varphi s_\varphi = \sin(2\varphi)$.

$$= -\frac{i\hbar}{4\pi} \left(i\sqrt{3}\, 2\pi + \int_0^{2\pi} d\varphi\, \cancel{\sin(2\varphi)} \right) = \frac{\sqrt{3}\hbar}{2}.$$

$\cancel{\sin(2\varphi)} \to 0$

VRTILNA KOLIČINA & OPERATORJI

Klasično : $\vec{L} = \vec{r} \times \vec{p}$ $\longrightarrow$ Kvantni operator $\hat{\vec{L}} = -i\hbar\, \hat{\vec{r}} \times \frac{\vec{d}}{d\vec{r}}$,

ali : $\hat{L}_i = -i\hbar\, \varepsilon_{ijk} x_j \frac{d}{dx_k}$.

sferične koordinate $\qquad$ kartezične koordinate

$x = r\cos\theta\cos\varphi, \quad y = r\cos\theta\sin\varphi, \quad z = r\sin\theta.$

$x_i = (x,y,z) \longrightarrow \xi_i = (r,\theta,\varphi), \quad J_{ij} = \frac{dx_i}{d\xi_j}$

$$\frac{d}{dx_i} = \frac{d}{d\xi_j}\frac{d\xi_j}{dx_i} = J^{-1}_{ij}\frac{d}{dx_j}$$

$\Downarrow$

$(L_x, L_y, L_z, L^2)(\theta,\varphi) \nearrow$

$$\hat{L}_x = i\hbar\left(\sin\varphi\,\frac{d}{d\theta} + \frac{\cos\varphi}{\tan\theta}\,\frac{d}{d\varphi}\right),$$

$$\hat{L}_y = i\hbar\left(-\cos\varphi\,\frac{d}{d\theta} + \frac{\sin\varphi}{\tan\theta}\,\frac{d}{d\varphi}\right),$$

$$\hat{L}_z = -i\hbar\,\frac{d}{d\varphi}\,,\quad \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left(\frac{d}{d\theta^2} + \cot\theta\,\frac{d}{d\theta} + \frac{1}{\sin^2\theta}\frac{d^2}{d\varphi^2}\right)$$

Sferični harmoniki Y_{lm} so lastne funkcije operatorjev $\hat{L}_z$ in $\hat{L}^2$ z lastnimi funkcijami:

$$\hat{L}_z Y_{lm} = \hbar m Y_{lm}\,,\quad \hat{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm}.$$

PRIMER : $$\psi = \frac{1}{\sqrt{2}}\left(Y_{10} + Y_{11}\right)$$

$$= \sqrt{\frac{3}{8\pi}}\left(c_\theta - \frac{1}{\sqrt{2}}\, s_\theta e^{i\varphi}\right).$$

Zanimali nas bodo $\langle L_i, L^2\rangle$, kar bomo napravili z a) eksplicitno integracijo in z b) lastnimi vrednostmi.

a) $\langle L_x\rangle$, $\hat{L}_x = +i\hbar\left(\sin\varphi\,\frac{d}{d\theta} + \frac{\cos\varphi}{\tan\theta}\,\frac{d}{d\varphi}\right)$

$$\langle L_x\rangle = \frac{1}{2}\int d\Omega\left(Y_{10}^* + Y_{11}^*\right) L_x \left(Y_{10} + Y_{11}\right)$$

$$= \frac{i\hbar 3}{8\pi}\int d\Omega\left(c - \frac{1}{\sqrt{2}}\, s\, e^{-i\varphi}\right)\Bigg(\frac{e^{i\varphi} - e^{-i\varphi}}{2i}\left(-s - \frac{1}{\sqrt{2}}\, c\, e^{i\varphi}\right)$$

$$+ \frac{e^{2i\varphi} + \cancel{e^{-i\varphi}}\,1}{2\,\cancel{\tan}\,\theta}\left(-\frac{i}{\sqrt{2}}\right)\cancel{\sin\theta}\;\cancel{e^{i\varphi}}\cos\theta\Bigg)$$

• velja: $\int_0^{2\pi} e^{in\varphi}\,d\varphi = 0\,,\ n \neq 0\,,\ \int_0^{2\pi} e^0\,d\varphi = 2\pi.$

• integriramo po φ in pomečemo $e^{in\varphi}$, $n \neq 0$

$$\langle L_x \rangle = \frac{3\cancel{i}\hbar}{8\pi} \int_{-1}^{1} dc \int_{0}^{2\pi} d\varphi \left(c - \frac{1}{\sqrt{2}} s e^{-i\varphi}\right)\left(\frac{e^{i\varphi}-e^{-i\varphi}}{2\cancel{i}}\left(-s - \frac{1}{\sqrt{2}} c e^{i\varphi}\right) + \frac{1+e^{2i\varphi}}{\cancel{i}\,2\sqrt{2}}\, c\right)$$

$$= \frac{3\hbar}{\cancel{8\pi}\,4} \int_{-1}^{1} dc \left(c\left(\frac{1}{2\sqrt{2}}c + \frac{1}{2\sqrt{2}}c\right) - \frac{1}{\sqrt{2}} s\left(-\frac{s}{2}\right)\right)\cdot \cancel{2\pi}$$

$$= \frac{3\hbar}{4}\,\frac{1}{2\sqrt{2}} \underbrace{\int_{-1}^{1} dc \left(\cancel{2}c^2 + 1 - \cancel{c^2}\right)}_{= 2 + \frac{2}{3} = \frac{8}{3}} = \frac{\hbar}{\sqrt{2}}.$$

• Podobno za: $\hat{L}_y = i\hbar\left(-c_\varphi \frac{d}{d\theta} + s_\varphi \frac{c}{s}\frac{d}{d\varphi}\right)$,

$$\langle L_y \rangle = \frac{i\hbar 3}{8\pi} \int d\Omega \left(c - \frac{1}{\sqrt{2}} s e^{-i\varphi}\right)\left(-\frac{e^{i\varphi}+e^{-i\varphi}}{2}\left(-s - \frac{1}{\sqrt{2}} c e^{i\varphi}\right) + \frac{e^{2i\varphi} - \cancel{e^{-i\varphi}}1}{2\cancel{i}}\,\frac{c}{\cancel{s}}\left(-\frac{\cancel{i}}{\sqrt{2}}\right)\cancel{s}\cancel{e^{i\varphi}}\right)$$

$$= \frac{i\hbar 3}{4\cancel{8\pi}}\cancel{2\pi} \int_{-1}^{1} dc \left(c\left(\frac{c}{2\sqrt{2}} + \frac{c}{\sqrt{2}\,2}\right) - \frac{s}{\sqrt{2}}\left(\frac{s}{2}\right)\right)$$

$$= \frac{3i\hbar}{2\sqrt{2}\,4} \underbrace{\int_{-1}^{1} dc\, \left(3c^2 - 1\right)}_{3\cdot\frac{2}{3} - 2 = 2 - 2 = 0.} = \underline{\underline{0}}.$$

$$\langle L_z \rangle = -\frac{i\hbar 3}{8\pi} \int_{-1}^{1} dc \int_{0}^{2\pi} d\varphi \left(c - \frac{1}{\sqrt{2}} s e^{-i\varphi}\right)\left(-\frac{i}{\sqrt{2}} s e^{i\varphi}\right)$$

$$= \cancel{-}\frac{\cancel{i}\hbar 3}{\cancel{8\pi}\,4}\cdot \frac{\cancel{i}}{\sqrt{2}^2}\cancel{2\pi} \underbrace{\int_{-1}^{1} (1-c^2)\, dc}_{2 - \frac{2}{3} = \frac{1}{3}} = \frac{3\hbar}{\sqrt{2}^2}\cdot\frac{1}{\cancel{3}} = \frac{\hbar}{2}.$$

b) Uporabimo zveze med lastnimi stanji:

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

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

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

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

$$\psi = \frac{1}{\sqrt{2}}\left(Y_{10}+Y_{11}\right)$$

$$\langle L_z\rangle = \frac{1}{2}\left(\int_\Omega Y_{10}^*\hat{L}_z Y_{10} + Y_{11}^*\hat{L}_z Y_{11}\right) = \frac{\hbar}{2}(0+1) = \frac{\hbar}{2},$$

$$\langle L^2\rangle = \frac{1}{2}\left(\int_\Omega Y_{10}^*\hat{L}^2 Y_{10} + Y_{11}\hat{L}^2 Y_{11}\right) = \frac{\hbar^2}{2}(1\cdot2+1\cdot2) = 2\hbar^2.$$

V obeh primerih smo izpustili mešane člene, ker $\delta_{l'l}=\delta_{10}=0$.

Pri $\langle L_{x,y}\rangle$ so ravno ti mešani členi različni od nič; dobimo:

$$\langle L_x\rangle = \frac{1}{2}\int_\Omega\left(Y_{10}^*\hat{L}_x Y_{11} + Y_{11}^*\hat{L}_x Y_{10}\right)$$

$$= \frac{1}{2}\frac{\hbar}{2}\Big(\underbrace{\sqrt{2-1(1-1)}}_{m'=0,\ m=1,\ \ominus} + \underbrace{\sqrt{2-0\cdot(0+1)}}_{m'=1,\ m=0,\ \oplus}\Big) = \frac{\hbar}{\sqrt{2}},$$

$$\langle L_y\rangle = \frac{1}{2}\int_\Omega\left(Y_{10}^*\hat{L}_y Y_{11} + Y_{11}^*\hat{L}_y Y_{10}\right)$$

$$= \frac{i\hbar}{4}\left(+\sqrt{2}-\sqrt{2}\right) = 0.$$