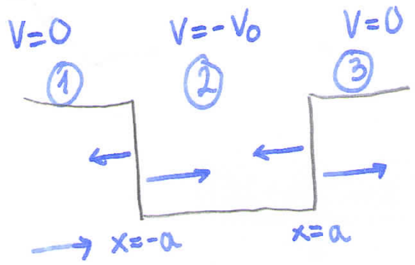
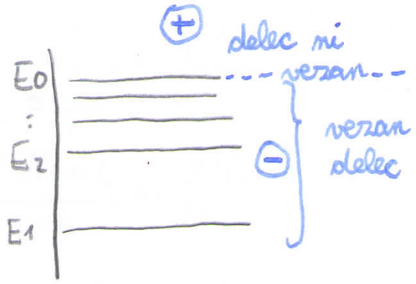
Delec v končni potencialni jami





1 $E > 0$!!! delec ni vezan

sipanje na jami => lahko izračunamo delež prepustnosti (η_{pre}) in odbitega (η_{od})

$$\eta_{od} = \frac{4k^2g^2}{(k^2-g^2)^2 \sin^2(2ga) + 4k^2g^2} \qquad g = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

$$\eta_{pre} = \frac{(k^2-g^2)^2 \sin^2(2ga)}{(k^2-g^2)^2 \sin^2(2ga) + 4k^2g^2}$$

2 $E < 0$; $E > -V_0$ delec je vezan

1,3 območje

$$\hat{H}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

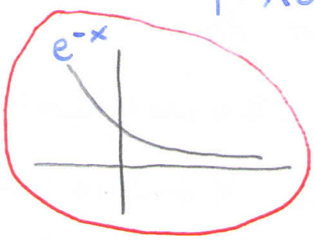
$$\boxed{E = -|E|}$$

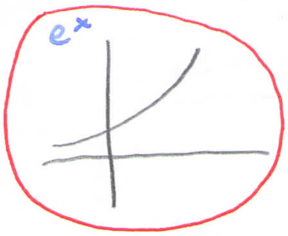
$$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} - \frac{2m|E|}{\hbar^2}\psi = 0 \qquad \chi^2 = \frac{2m|E|}{\hbar^2}$$

$$\frac{\partial^2\psi}{\partial x^2} - \chi^2\psi = 0$$

$$\psi = Ae^{-\chi x} + Be^{\chi x} \Rightarrow \psi_1 = Be^{\chi x} \quad (1)$$





$$\psi_3 = Ae^{-\chi x} \quad (3)$$

(2) območje $\hat{H}\psi = E\psi$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

$$\boxed{\begin{aligned} V &= -V_0 \\ E &= -|E| \end{aligned}}$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(V_0 - |E|)\psi = 0 \qquad k^2 = \frac{2m(V_0-|E|)}{\hbar^2}$$

$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0$$

v pot. jami (V_0)
~~vezani delci~~ (~~$E<0$~~)

sin, cos ...	~~delci~~
e ...	~~valovanje~~

~~nevezani delci~~ (~~$E>0$~~)
izven pot. jame ($V=0$)

$$\psi_2 = C\sin kx + D\cos kx$$

zveznost in odvodljivost:

$$\psi_1(-a) = \psi_2(-a) \quad 1$$
$$\psi_2(a) = \psi_3(a) \quad 2$$
$$\frac{\partial\psi_1}{\partial x}(-a) = \frac{\partial\psi_2}{\partial x}(-a) \quad 3$$
$$\frac{\partial\psi_2}{\partial x}(a) = \frac{\partial\psi_3}{\partial x}(a) \quad 4$$

$\underline{1}$ $Be^{-\varkappa a} = -C\sin ka + D\cos ka$

$\Rightarrow \underline{2}$ $C\sin ka + D\cos ka = Ae^{-\varkappa a}$

odvodi:
$$\begin{cases} \dfrac{\partial\psi_1}{\partial x} = B\varkappa e^{\varkappa x} \\ \dfrac{\partial\psi_2}{\partial x} = Ck\cos kx - Dk\sin kx \\ \dfrac{\partial\psi_3}{\partial x} = -A\varkappa e^{-\varkappa x} \end{cases}$$

$\underline{3}$ $B\varkappa e^{-\varkappa a} = Ck\cos ka + Dk\sin ka$

$\underline{4}$ $Ck\cos ka - Dk\sin ka = -A\varkappa e^{-\varkappa a}$

$\underline{1}$ pomnožimo s $\varkappa$ in odštejemo $\underline{3}$:

$$0 = Ck\cos ka + C\varkappa\sin ka + Dk\sin ka - D\varkappa\cos ka$$

$\underline{2}$ pomnožimo s $\varkappa$ in seštejemo z $\underline{4}$:

$$C\varkappa\sin ka + Ck\cos ka + D\varkappa\cos ka - Dk\sin ka = 0$$

seštejemo obe:

$$0 = 2C\varkappa\sin ka + 2Ck\cos ka$$
$$0 = 2C(\varkappa\sin ka + k\cos ka) \quad /:2$$
$$0 = C(k\cos ka + \varkappa\sin ka)$$

I. $C=0$:

$D(k\sin ka - \varkappa \cos ka) = 0$

Ia. $D=0$:

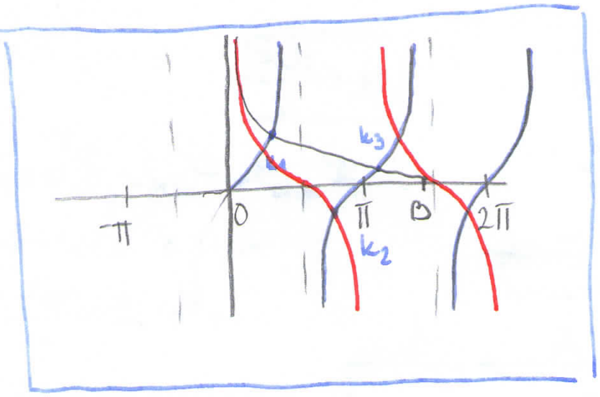
$\psi_2 = 0$
$\psi_1 = 0$ } ni fizikalna rešitev
$\psi_3 = 0$

Ib. $k\sin ka - \varkappa\cos ka = 0$

$k\sin ka = \varkappa\cos ka \quad / : k\cos ka$

$$\boxed{\begin{gathered} k^2 = \underbrace{\frac{2mV_0}{\hbar^2}}_{\beta^2} - \underbrace{\frac{2m|E|}{\hbar^2}}_{\varkappa^2} \\ \varkappa^2 = \beta^2 - k^2 \\ \varkappa = \sqrt{\beta^2 - k^2} \end{gathered}}$$

$$\tan ka = \frac{\sqrt{\beta^2-k^2}}{k}$$



II. $k\cos ka + \varkappa\sin ka = 0$

IIa. $D=0$

$k\cos ka + \varkappa\sin ka = 0$

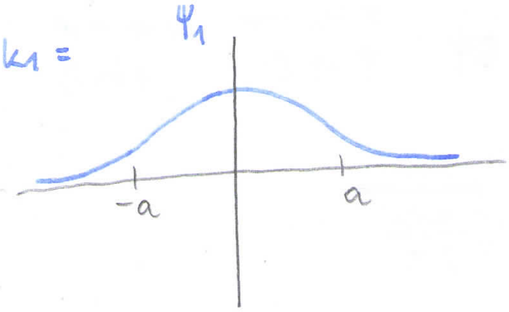
$k\cos ka = -\varkappa\sin ka \quad / : k\sin ka$

$$\operatorname{ctg} ka = -\frac{\sqrt{\beta^2-k^2}}{k}$$

IIb. $k\sin ka - \varkappa\cos ka = 0$

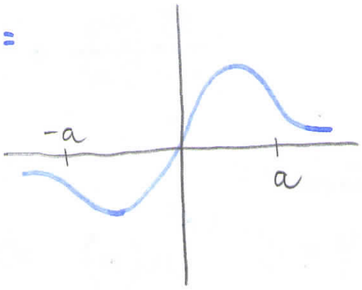
$k=0$ ni fiz. rešitev

$k_1 =$



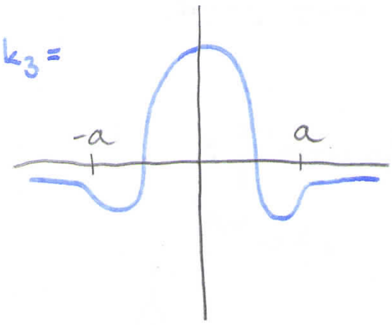
SODA f

$k_2 =$

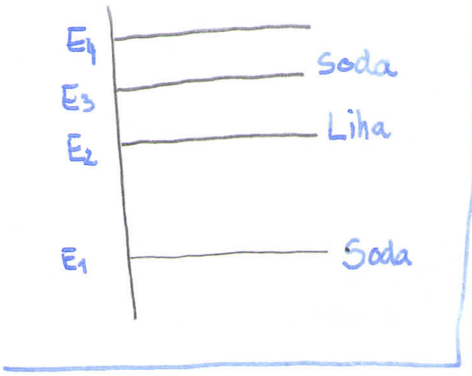


LIHA f

$k_3 =$



SODA f

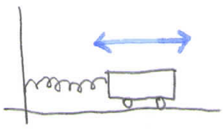


večji imamo B, več vezanih stanj imamo;
na grafu je B dlje na x-osi (proti desni)

večji imamo a, več vezanih stanj imamo;
na grafu se tan krči

Ne glede na širino in globino jame imamo VSAJ ENO VEZANO STANJE.

Harmonski oscilator



$x = x_0 \sin \omega t$

$v = v_0 \cos \omega t$

$$E = \frac{1}{2}kx^2 + \frac{1}{2}mv^2 = \underline{\frac{1}{2}kx_0^2}$$

$$dw = A \cdot dt \qquad \boxed{dt = \frac{dx}{v}}$$

$$dw = A \frac{dx}{v}$$

$$\cancel{\frac{1}{2}} mv^2 + \cancel{\frac{1}{2}} kx^2 = \cancel{\frac{1}{2}} kx_0^2$$

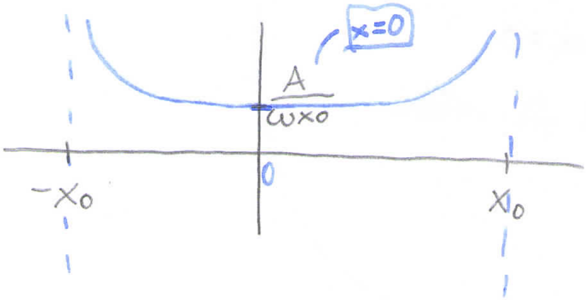
$$mv^2 = kx_0^2 - kx^2$$

$$v^2 = \frac{k(x_0^2 - x^2)}{m} \qquad \frac{k}{m} = \omega^2$$

$$v = \omega\sqrt{x_0^2 - x^2}$$

$$dw = A \frac{dx}{\omega\sqrt{x_0^2 - x^2}}$$

$$\frac{dw}{dx} = \frac{A}{\omega} \cdot \frac{1}{\sqrt{x_0^2 - x^2}}$$



$\boxed{V = \frac{1}{2}kx^2}$ v kv. svetu

$$\hat{H}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi$$

$x \to \infty$, $V \to -\infty$, $\psi \to 0$

$x \to -\infty$, $V \to -\infty$, $\psi \to 0$

Gaussova f:

$y = e^{-ax^2}$

izračunamo:

$$\psi = e^{-ax^2} u(x) \Rightarrow a = \sqrt{\frac{km}{2\hbar}}$$

Dobimo Hermitove polinome:

$$E_n = \hbar\omega\left(n+\tfrac{1}{2}\right) \qquad n \in \{0,1,2,\dots\}$$

$$u_n(t) = H_n(t) \qquad \psi_n = \underline{N_n}\, e^{-\frac{m\omega^2}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)$$

$$t = \sqrt{4\alpha}\,x$$

NORMALIZACIJSKA KONST.

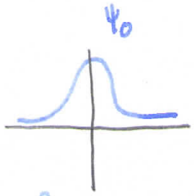
$H_0 = 1$

$H_1 = 2x \qquad H_{n+1} = 2x H_n - 2nH_{n-1}$

$H_2 = 2x\cdot 2x - 2\cdot 1\cdot 1 = 4x^2-2$

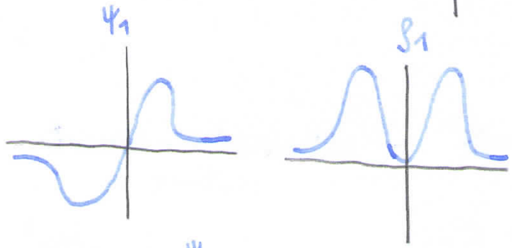
$\boxed{n=0}$ - osnovno stanje

$E_0 = \frac{1}{2}\hbar\omega \qquad \underline{\psi_0 \propto e^{-ax^2}}$

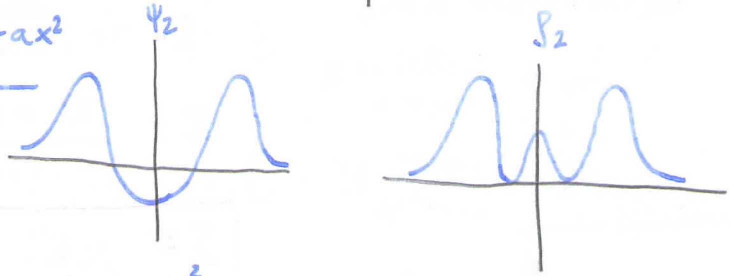


BOHROV PRINCIP KORESPODENCE

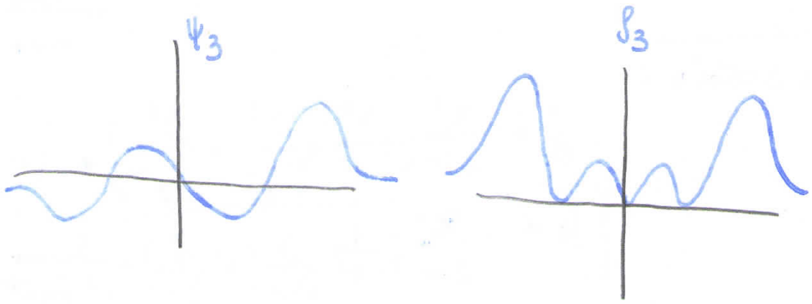
$\underline{\psi_1 \propto x e^{-ax^2}}$



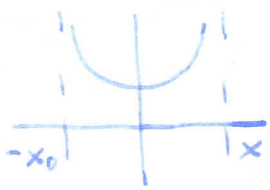
$\underline{\psi_2 \propto (4x^2-2)e^{-ax^2}}$



$\underline{\psi_3 \propto (8x^3-12x)e^{-ax^2}}$



Z večanjem kv. števila ($n=0,1,2\dots$) se bližamo



Vrtilna količina
(PONOVITEV)

$[\hat{L}_x, \hat{L}_z] \neq 0$

$[\hat{L}_x, \hat{L}^2] = [\hat{L}_y, \hat{L}^2] = [\hat{L}_z, \hat{L}^2] = 0$

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

$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\vartheta} \frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)$

$$\boxed{\begin{aligned} \hat{L}_z Y_{em} &= m\hbar Y_{em} \\ \hat{L}^2 Y_{em} &= l(l+1)\hbar^2 Y_{em} \end{aligned}}$$

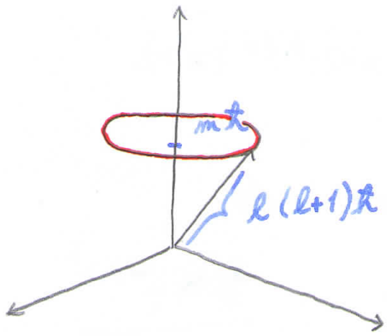
$m\hbar$ - velikost komponente L_z

$l(l+1)\hbar^2$ - velikost kvadrata vrt. količine

$\langle \hat{L}^2 \rangle = l(l+1)\hbar^2$

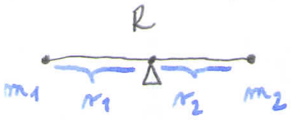
$\langle \hat{L}_z \rangle = m\hbar$

$$\boxed{|\vec{L}| = \hbar\sqrt{l(l+1)}}$$



če poznamo kv. št. l, je $-l \leq m \leq l$

Togi rotator



$I = m_1 r_1^2 + m_2 r_2^2$ - vztrajnostni moment sistema

$r_1(m_1+m_2) = R m_2$

$r_1 = \frac{m_2}{m_1+m_2} R$

$r_2 = \frac{m_1}{m_1+m_2} R$

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

$I = \frac{R^2 m_1 m_2 \cancel{(m_1+m_2)}}{(m_1+m_2)^{\cancel{2}}}$

$$\boxed{I = \mu R^2}$$

reducirana masa

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

KLASIČNI DELEC:

$W_k = \frac{\Gamma^2}{2I}$ $\quad \Gamma$ - vrtilna količina

Zapišemo Schrödingerjevo stac. enačbo:

$\hat{H}\Psi = E\Psi$

$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\vec{r})$

$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right) + V$

v sferičnih koordinatah

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\cancel{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)} + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\,\frac{\partial\psi}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right) + V(\vec{r})\psi = E\psi$$

razdalja od izhodišča :
$r = R$, je konst. => $\boxed{\frac{\partial\psi}{\partial r} = 0}$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{1}{R^2}\left(\cancel{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\,\frac{\partial\psi}{\partial\vartheta}\right)} + \frac{1}{\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right) + V\psi$$

$mR^2 = I$

$\hat{H} = \frac{\hat{L}^2}{2I} + V$

zamislimo si delec, ki kroži po ravnini : ϑ se ne spreminja, konst =>

$\boxed{\frac{\partial\psi}{\partial\vartheta} = 0}$ $\quad \vartheta = 90^\circ$

$$\hat{H}\psi = \frac{-\hbar^2}{\underset{\Downarrow\;I}{2mR^2}}\left(\frac{1}{\underset{\Downarrow\;1}{\sin^2\vartheta}}\frac{\partial^2\psi}{\partial\varphi^2}\right) + \cancel{V\psi}$$

prosto kroženje => $\boxed{V=0}$

$$\hat{H}\psi = -\frac{\hbar^2}{2I}\frac{\partial^2\psi}{\partial\varphi^2} = E\psi \quad \Big/ \cdot -\frac{2I}{\hbar^2}$$

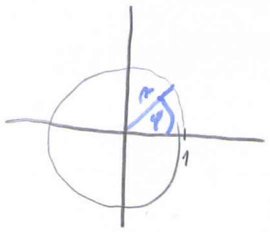
$$\frac{\partial\psi}{\partial\varphi^2} + m^2\psi = 0 \qquad m^2 = \frac{2IE}{\hbar^2}$$

$$\psi = Ae^{im\varphi} + Be^{-im\varphi}$$

$\boxed{\psi(\varphi + 2\pi) = \psi(\varphi)}$

$$\underbrace{Ae^{im(\varphi+2\pi)}}_{e^{im\varphi}\cdot e^{im2\pi}} + Be^{-im(\varphi+2\pi)} = Ae^{im\varphi} + Be^{-im\varphi} \qquad \boxed{m \in \mathbb{N}}$$

=> $e^{im2\pi} = 1$


$z = a + bi = r\cdot e^{i\varphi}$

$m2\pi = 0 + 2\pi n$

$n \in \mathbb{Z}$

$m \in \mathbb{Z}$

$$E_m = \frac{m^2\hbar^2}{2I}$$

$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$; $H = \frac{\hat{L}_z^2}{2I}$ => $\boxed{[\hat{L}_z, \hat{H}] = 0}$

$\psi = Ae^{im\varphi}$ - lastna funkcija za $\hat{H}$

$$\hat{L}_z\psi = -i\hbar\frac{\partial}{\partial\varphi}Ae^{im\varphi} = -i\hbar Ae^{im\varphi}(im) = m\hbar Ae^{im\varphi} = m\hbar\psi$$

$\langle\hat{L}_z\rangle = m\hbar$

$$\boxed{E_m = \frac{\langle\hat{L}_z\rangle^2}{2I}}$$

splošno vrtenje, $V=0$:

$$\hat{H} = \frac{\hat{L}^2}{2I} \qquad \hat{L}^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}$$

$$[\hat{L}^2, \hat{H}] = 0 \qquad \hat{H} Y_{lm} = \frac{\hat{L}^2}{2I} Y_{lm} = \frac{l(l+1)\hbar^2}{2I} Y_{lm}$$

$$[\hat{L}_z, \hat{H}] = 0$$

$$\boxed{E_l = \frac{l(l+1)\hbar^2}{2I}} \qquad -l \le m \le l$$

l	m	E
0	0	$E=0$ – delec se ne vrti
1	-1	$E_1 = \frac{1 \cdot 2 \cdot \hbar^2}{2I} = \frac{\hbar^2}{I}$ } 3 degenerirana stanja: Y_{1-1}, Y_{10}, Y_{11}
	0	
	1	
l	$-l, \dots l$	$E = \frac{\hbar^2 (l+1) l}{2I}$ deg. stanje: $(2l+1)$

orbitale:

$$Y_{00} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2\pi}} \longrightarrow$$

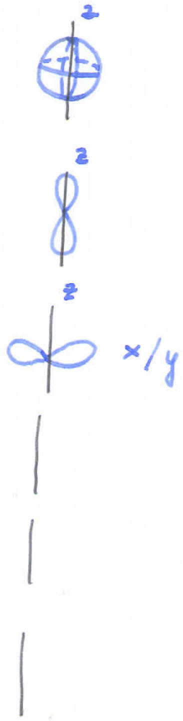
$$Y_{10} = \sqrt{\frac{2}{3}} \cos\vartheta \frac{1}{\sqrt{2\pi}} \longrightarrow$$

$$Y_{1\pm1} = \sqrt{\frac{3}{4}} \sin\vartheta \frac{1}{\sqrt{2\pi}} e^{\pm i\varphi} \longrightarrow$$

$$Y_{20} = \sqrt{\frac{5}{8}} (3\cos^2\vartheta - 1) \frac{1}{\sqrt{2\pi}} \longrightarrow$$

$$Y_{2\pm1} = \sqrt{\frac{15}{4}} \sin\vartheta \cos\vartheta \frac{1}{\sqrt{2\pi}} e^{\pm i\varphi} \longrightarrow$$

$$Y_{2\pm2} = \sqrt{\frac{15}{16}} \sin^2\vartheta \frac{1}{\sqrt{2\pi}} e^{\pm 2i\varphi} \longrightarrow$$



$$Y_{lm} = \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}} \, P_l^{|m|}(\cos\vartheta)$$

P_l → modificiran Legendrov polinom

$$\boxed{\langle Y_{lm} | Y_{l'm'} \rangle = \int_0^{\pi} d\vartheta \int_0^{2\pi} d\varphi \, Y^*_{lm} Y_{l'm'} \sin\vartheta}$$

$$\langle Y_{lm} | Y_{l'm'} \rangle = \delta_{ll'} \delta_{mm'} \qquad \psi = A e^{im\varphi} \rightarrow \text{lastna f. za } \hat{H}$$