QMI-cv8 – sférické harmoniky

pozn: $Y_{lm}(\theta,\varphi)$ ... L^2 ... $p_l(x,y,z)$ ... $f(r)$

r l r r^{-l}

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

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

$z = r\cos\theta$

$p_l(\lambda x, \lambda y, \lambda z) = \lambda^l p_l(x,y,z)$ ... $\lambda = r$

$p_l(x,y,z) = p_l(\theta,\varphi)\, r^l$

$$\boxed{Y_{lm}(\theta,\varphi) = p_l(x,y,z)\, r^{-l}}$$

nebo $Y_{lm}(\theta,\varphi) = p_l$ na $\vec{x} \in S_2$ tj. $x^2+y^2+z^2=1$

ÚLOHA 1

- $l=0$ ... $Y_{00}(\theta,\varphi) = C$

$1 = \int |Y_{00}|^2 \, d\Omega = C^2 \int_{S_2} 1\, d\Omega = 4\pi C^2 \rightarrow C = \frac{1}{\sqrt{4\pi}}$

- $l=1$ Y_{11} Y_{1-1} Y_{10} ... $p_l(x,y,z) = ax + by + cz$

$\Delta p_l = 0$

$\hat{L}_+ Y_{11} = 0$

$\hat{L}_+ = \hat{L}_x + i\hat{L}_y = -i\hbar\left[y\partial_z - z\partial_y + iz\partial_x - ix\partial_z\right]$

$z \to y$ $y \to (-z)$ $x \to (iz)$ $z \to (-ix)$

$\hat{L}_+ p_l = 0$

$cy - bz + iaz - cix = 0$ identicky $\forall\, x,y,z$

$\Leftrightarrow\ \boxed{(-ci)x + cy + (ia-b)z = 0}$

$-ic = 0$, $c = 0$, $b = ia$, $a = 1$

$$\boxed{Y_{11} = N(x+iy)\frac{1}{r}} \qquad \boxed{x^2+y^2+z^2=1}$$

$x \to \frac{x}{r}$ $y \to \frac{y}{r}$

$\hat{L}_- = -i\hbar\left[y\partial_z - z\partial_y - iz\partial_x + ix\partial_z\right]$ $\quad a = N\cdot 1 \quad c = 0$
$b = N\cdot i$

$L_- Y_{11} = -i\hbar k^* = -i\hbar(-ia - b)z = -2izN - i\hbar = -2z\hbar N$

$\underset{\cdot N}{\overset{1}{}}\ \underset{i\cdot N}{}$ $\qquad = \sqrt{2}\hbar Y_{00}$

$$\boxed{L_\pm |l\,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}\,|l\ m\pm 1\rangle}$$
$\quad 1\ 1\ 0 \qquad 2\cdot 1$

$Y_{00} = -\sqrt{2}\,z\cdot N$

dodomé ... $Y_{1-1} = N\cdot(x - iy)$

Souhrn: $\cdot\ Y_{11} = N(x+iy)$

$Y_{10} = -\sqrt{2}Nz$

$\cdot\ Y_{1-1} = -N(x+iy)$

N ?
$x = \cos\varphi\sin\theta$
$z = 1\cos\theta$

$f(x,y,z) = x$ na S_2 $\quad \int f^2 d\Omega$

$$\int_{S_2} x^2 d\Omega = \int_{S_2} y^2 d\Omega = \int_{S_2} z^2 d\Omega = \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_0^\pi \underbrace{\sin\theta d\theta}_{dz} \cos^2\theta \qquad z = \cos\theta$$

$$= 2\pi\int_{-1}^1 z^2 dz = 4\pi\int_0^1 z^2 dz = \frac{4\pi}{3}$$

$$\int_0^1 x^n dx = \frac{1}{n+1}$$

$$\int |Y_{10}|^2 d\Omega = 2N^2\int z^2 d\Omega = 2N^2\frac{4\pi}{3} = \qquad N = \sqrt{\frac{3}{8\pi}}$$

závěr: $\underbrace{Y_{10} = +\sqrt{\frac{3}{4\pi}}\frac{z}{r}}_{(-1)}$ $\qquad Y_{11} = \sqrt{\frac{3}{8\pi}}\frac{(x+iy)}{r}\cdot(-1)$

$Y_{1-1} = -\sqrt{\frac{3}{8\pi}}\frac{(x-iy)}{r}\cdot(-1)$

fázová konvence Y_{l0} ... severní pól $Y_{l0} > 0$ $\qquad z = 1$
$\theta = 0$ φ libovolné $\qquad \cos\theta = 1$

$\boxed{\ell = 2}$ $\quad Y_{22} \quad Y_{21} \quad Y_{20} \quad Y_{2-1} \quad Y_{2-2} \qquad p_2(x,y,z)$

$$p_2(x,y,z) = ax^2 + by^2 + cz^2 + \alpha yz + \beta xz + \gamma xy$$

$$\Delta p = 2a + 2b + 2c \ \dots \qquad a+b+c = 0 \qquad c = -a-b$$

$L_+ Y_{22} = 0$

$\forall x, y, z$

	x^2	y^2	z^2	yz	xz	xy
p_2	a	b	$-a-b$	α	β	γ
$z \to y$		α		$-2(a+b)$		β
$y \to -z$			$-\alpha$	$-2b$	$-\gamma$	
$x \to +iz$				$i\gamma$	$2ia$	$-\alpha i$
$z \to -ix$	$-\beta i$		$+\beta i$		$2i(a+b)$	
	$\cancel{-\beta i}$	$\cancel{\alpha}$	$\cancel{-\alpha+\beta i}$	$-2(a+b)$ $-2b$ $+\gamma i$	$-\gamma$ $+2ia$ $+2i(a+b)$	$\beta - \alpha i$
	$= 0$	$= 0$	$= 0$	$= 0$	$= 0$	$= 0$

$$\left.\begin{aligned} -2a - 4b + i\gamma &= 0 \\ -\gamma + 2i(2a+b) &= 0 \end{aligned}\right\} \to \quad \begin{aligned} b &= -a \\ \gamma &= 2ia \end{aligned}$$

$$Y_{22} = ax^2 + 2ia\,xy - ay^2 = a(x+iy)^2 = \sin^2\theta\, e^{2i\varphi}$$

$x = \cos\varphi \sin\theta$, $y = \sin\varphi\sin\theta$

$\downarrow$

Y_{21}

Y_{20}

$$\sin^{2\,2} = (1-\cos^2)^2$$

$$\int |Y_{22}|^2 d\Omega = \int_0^{2\pi}\int_0^{\pi} (\sin\theta)^4 \underbrace{\sin\theta\, d\theta}_{d\cos\theta}\, d\varphi = 4\pi \int_0^1 (1-z^2)^2 dz$$

z

$$4\pi \int_0^1 (1-2z^2+z^4)\,dz = 4\pi \cdot \frac{8}{15} \to \sqrt{\frac{15}{32\pi}}$$

$$\frac{1}{1} - 2\frac{1}{3} + \frac{1}{5} = \frac{15-10+3}{15}$$

pref

ÚLOHA 2 $\quad \psi(\vec{r}) = (x+y+3z)\, f(r)$

(1) ? je vl. fce $\hat{L}^2$? ... l ?

(2) jaká je p_m ... $\hat{L}_z$ ... $\hbar m$

$\boxed{\text{Pref}}$ je homogfoly st $l=1$ $\Delta p = 0$ $\;$ $r\,l\,m$

ti $\longrightarrow$ ψ je vl fcí L^2 ... $\hbar^2 l(l+1)$

$l=1$

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(2) ψ -- vl. podpr $l=1$

$$\psi_\Omega = \left(a\, Y_{11} + b\, Y_{10} + c\, Y_{1-1}\right)$$ radiální fce

úhl. $\dfrac{x+y+3z}{r} =$

h_0

$\sqrt{\;\cdot/\cdot\;}\, Y_{10} = \sqrt{2}\, z$

$h_+ = \sqrt{\frac{8\pi}{3}}\, Y_{11} = -x - iy$

$h_- = \sqrt{\;\cdot/\cdot\;}\, Y_{1-1} = x - iy$

$h_+ + h_- = -2iy$

$2x = h_- - h_+$

$$\psi_\Omega = \frac{3}{\sqrt{2}} h_0 + \frac{h_+ + h_-}{-2i} + \frac{h_- - h_+}{2}$$

$$\sqrt{\frac{3}{8\pi}}\,\Psi_\Omega = \underbrace{\frac{3}{\sqrt{2}}}\,Y_{10} + Y_{11}\underbrace{\left(-\frac{1}{2}+\frac{i}{2}\right)} + Y_{1-1}\underbrace{\left(\frac{1}{2}+\frac{i}{2}\right)}$$

$$N^2 = \frac{9}{2} + \frac{2}{4} + \frac{2}{4} = \frac{11}{2}$$

$$\bar{\Psi}_\Omega^{\text{ - normovana}} = \frac{\Psi_\Omega}{N} = \sqrt{\frac{2}{11}}\left(\frac{3}{\sqrt{2}}Y_{10} + \left(\frac{i}{2}-\frac{1}{2}\right)Y_{11} + \left(\frac{i}{2}+\frac{1}{2}\right)Y_{1-1}\right)$$

vl. fce L_z $\quad m=0 \quad m=1 \quad m=-1$

$$\bar{\Psi}_\Omega = c_0 Y_{10} + c_+ Y_{11} + c_- Y_{1-1}$$

$$p_m = |c_m|^2 \qquad \sum p_m = 1$$

$$\boxed{p_0 = c_0^2 = \frac{2}{11}\cdot\frac{9}{2} = \frac{18}{22} \qquad p_{\pm 1} = \frac{2}{11}\,\frac{2}{4} = \frac{2}{22}}$$

$m=0$ $\quad \frac{9}{11} \quad$ $m=\pm 1$ $\quad \frac{1}{11}$