mom. lybashi basics

2022-UKM-TP5

$$\vec{L} = \vec{r} \times \vec{p} = -i\hbar\Big(\underbrace{y\frac{d}{dz} - z\frac{d}{dy}}_{\hat{L}_x},\ \underbrace{z\frac{d}{dx} - x\frac{d}{dz}}_{\hat{L}_y},\ \underbrace{x\frac{d}{dy} - y\frac{d}{dx}}_{\hat{L}_z}\Big) \qquad (3D)$$

$$[\hat{L}_x, \hat{L}_y] = -\hbar^2\Big[y\frac{d}{dz} - z\frac{d}{dy},\ z\frac{d}{dx} - x\frac{d}{dz}\Big] = -\hbar^2\Big[y\frac{d}{dz}, z\frac{d}{dx}\Big] - \hbar^2\Big[-z\frac{d}{dy}, x\frac{d}{dz}\Big]$$

$$= -\hbar^2\Big(y\frac{d}{dz}z\frac{d}{dx} - z\frac{d}{dx}y\frac{d}{dz}\Big) + \hbar^2\Big(z\frac{d}{dy}x\frac{d}{dz} - x\frac{d}{dz}z\frac{d}{dy}\Big)$$

$$= -\hbar^2 y\frac{d}{dx}\Big(\frac{d}{dz}z - z\frac{d}{dz}\Big) + \hbar^2\frac{d}{dy}x\Big(z\frac{d}{dz} - \frac{d}{dz}z\Big)$$

$$\Big(\frac{d}{dz}z - z\frac{d}{dz}\Big)f(z) = \frac{d}{dz}zf(z) - z\frac{df}{dz} = f(z) + z\frac{df}{dz} - z\frac{df}{dz} = f(z) = 1\cdot f(z)$$

$$= -\hbar^2 y\frac{d}{dx} - \hbar^2\frac{d}{dy}x = i\hbar\, i\hbar\Big(y\frac{d}{dx} - \frac{d}{dy}x\Big) = i\hbar(y p_x - p_y x) = i\hbar L_z$$

sign?

$[x, p_x], \dots \quad [x, L_y], \dots \quad [p_x, L_y \dots] \quad [L_x, L_y]$

$$\vec{L} = \vec{r} \times \vec{p} = (y p_z - z p_y,\ z p_x - x p_z,\ x p_y - y p_x)$$

$$[x, p_x]f = x p_x f - p_x x f = x p_x f - (-i\hbar)\frac{d}{dx}x f = x(-i\hbar)\frac{df}{dx} + i\hbar f + i\hbar x\frac{df}{dx}$$

$$= i\hbar f$$

$$\Rightarrow [x, p_x] = i\hbar$$

$$[x, L_x] = [x, y p_z - z p_y] = 0$$

$$[x, L_y] = [x, z p_x - x p_z] = [x, z p_x] - \underbrace{[x, x p_z]}_{=0} = z[x, p_x] = i\hbar z$$

$$[x, L_z] = [x, x p_y - y p_x] = \underbrace{[x, x p_y]}_{=0} - [x, y p_x] = -y[x, p_x] = -i\hbar y$$

$$[p_x, L_y] = [p_x, z p_x - x p_z] = \underbrace{[p_x, z p_x]}_{=0} - [p_x, x p_z] = -p_z[p_x, x] = i\hbar p_z$$

$$[L_x, L_y] = [y p_z - z p_y,\ z p_x - x p_z] = [y p_z, z p_x] + [z p_y, x p_z] =$$

$$= y p_x \underbrace{[p_z, z]}_{\to -i\hbar} + p_y x \underbrace{[z, p_z]}_{\to i\hbar} = y p_x(-i\hbar) + i\hbar p_y x = i\hbar(\underbrace{x p_y - y p_x}_{L_z})$$

$$= i\hbar L_z$$

⋮

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$[L^2, L_x] = [L_x^2 + L_y^2 + L_z^2, L_x] = [L_y^2, L_x] + [L_z^2, L_x]$$

$$= L_y^2 L_x - L_x L_y^2 + L_z^2 L_x - L_x L_z^2$$

$$= L_y^2 L_x - L_y L_x L_y + L_y L_x L_y - L_x L_y L_y + L_z L_z L_x - L_z L_x L_z + L_z L_x L_z - L_x L_z^2$$

$$= L_y\underbrace{[L_y, L_x]}_{-i\hbar L_z} + \underbrace{[L_y, L_x]}_{-i\hbar L_z}L_y + L_z\underbrace{[L_z, L_x]}_{i\hbar L_y} + \underbrace{[L_z, L_x]}_{i\hbar L_y}L_z$$

$$= -2i\hbar L_y L_z + 2i\hbar L_y L_z = 0$$

2012 - UKM-Tab.6

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

norm: $$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \, \frac{1}{\sqrt{4\pi}}\cdot\frac{1}{\sqrt{4\pi}} = \frac{1}{4\pi}\int_0^\pi d\theta \sin\theta \underbrace{\int_0^{2\pi} d\phi \, 1}_{2\pi}$$

$$= \frac{1}{2}\int_0^\pi d\theta \sin\theta = \frac{1}{2}\left[-\cos\theta\right]_0^\pi = -\frac{1}{2}\left[-1-1\right] = 1$$

$$\int_0^\pi d\theta \sin\theta \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \frac{3}{4\pi}\cos^2\theta = \frac{3}{2}\int_0^\pi d\theta \sin\theta \cos^2\theta$$

$$= \frac{3}{2}\int_{1}^{-1} (-t^2)\,dt = \frac{3}{2}\int_{-1}^{1} t^2\, dt \qquad \begin{array}{l} \cos\theta = t \\ -\sin\theta d\theta = dt \end{array}$$

$$= \frac{3}{2}\,\frac{1}{3}\, t^3\Big|_{-1}^{1} = 1$$

$$Y_0^0\, Y_0^1 = \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \, \frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{4\pi}}\cos\theta =$$

$$= \frac{\sqrt{3}}{4\pi}\cdot 2\pi \cdot \int_0^\pi d\theta \sin\theta\cos\theta = \frac{\sqrt{3}}{2}\cdot\int_{-1}^{1} t\, dt = \frac{\sqrt{3}}{2}\,\frac{t^2}{2}\Big|_{-1}^{1} = 0$$

$$\to 0$$

$$Y_0^1\, Y_1^1 = -\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \, \frac{3}{4\pi\sqrt{2}}\cos\theta \sin\theta \, e^{i\phi}$$

$$L_z Y_1^1 = -i\hbar\frac{\partial}{\partial\phi}\left(-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\right) = -i\hbar(i)\underbrace{\left(-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\right)}_{Y_1^1}$$

$$= \hbar\, Y_1^1 \quad \text{OK}$$

$$L^2 Y_1^1 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\left(-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\right)$$

$$= \hbar^2\sqrt{\frac{3}{8\pi}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\cos\theta\, e^{i\phi} + \frac{1}{\sin^2\theta}(-)\,\cancel{\sqrt{\tfrac{3}{8\pi}}}\sin\theta\, e^{i\phi}\right]$$

$$= \hbar^2\sqrt{\frac{3}{8\pi}}\left[\frac{1}{\sin\theta}e^{i\phi}\left(\cos^2\theta - \sin^2\theta\right) - \frac{1}{\sin\theta}e^{i\phi}\right]$$

moment hybnosti  2022-ukn-TS:1

$L^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle \qquad L_z|lm\rangle = \hbar m|lm\rangle$

$\langle lm|l'm'\rangle = \delta_{ll'}\delta_{mm'}$

$l = 0, 1, 2, \dots \qquad m = \underbrace{l, l-1, \dots -l}_{2l+1 \text{ stavů / vl. vektorů}}$

dim $\infty$

$|00\rangle, |11\rangle, |10\rangle, |1-1\rangle, |22\rangle, |21\rangle, |20\rangle, |2-1\rangle, |2-2\rangle, \dots$

$\langle lm|L^2|l'm'\rangle = \langle lm|\hbar^2 l'(l'+1)|l'm'\rangle = \hbar^2 l'(l'+1)\langle lm|l'm'\rangle = \hbar^2 l(l+1)\delta_{ll'}\delta_{mm'}$

$\langle lm|L_z|l'm'\rangle = \cancel{\langle lm|\hbar^2 \dots}$

$\langle lm|\hbar m'|l'm'\rangle = \hbar m'\langle lm|l'm'\rangle = \hbar m'\delta_{ll'}\delta_{mm'}$

$\delta_{ll'}$ - diagonální bloky v $l$

$\delta_{mm'}$ - diagonální v $L_z$ ($m$)

$$l(l+1) \begin{cases} l=0 \to 0 \\ l=1 \to 2 \\ l=2 \to 6 \end{cases}$$

$$\to L^2 = \hbar^2 \begin{pmatrix} 0 & \emptyset & \emptyset & \\ \emptyset & \begin{matrix} 2&0&0\\0&2&0\\0&0&2 \end{matrix} & \emptyset & \emptyset \\ \emptyset & \emptyset & \begin{matrix} 6&0&0&0&0\\0&6&0&0&0\\0&0&6&0&0\\0&0&0&6&0\\0&0&0&0&6 \end{matrix} & \dots \\ & \emptyset & & \ddots \end{pmatrix} \qquad L_z = \hbar \begin{pmatrix} 0 & & \emptyset \\ & \begin{matrix} 1&0&0\\&0&\\0&&-1 \end{matrix} & & \\ & & \begin{matrix} 2&&&&\\&1&&\emptyset&\\&&0&&\\&\emptyset&&-1&\\&&&&-2 \end{matrix} & \\ \emptyset & & & \begin{matrix} 3 & \\ & 2 \dots \end{matrix} \end{pmatrix}$$

---

$L_+|lm\rangle = \hbar\sqrt{l(l+1) - m(m+1)}\,|l\,m+1\rangle$

$\langle l'm|L_+|l'm'\rangle = \hbar\sqrt{l'(l'+1) - m'(m'+1)}\,\underbrace{\langle lm|l'm'+1\rangle}_{\delta_{ll'}\delta_{m,m'+1}}$

pro $l = 0 \Rightarrow m = 0 \qquad L_+ = (0)$

$$l = 1 \to \begin{array}{c|ccc} m \backslash m' & 1 & 0 & -1 \\ \hline 1 & 0 & \emptyset & \emptyset \\ 0 & 0 & \emptyset & \emptyset \\ -1 & 0 & 0 & \emptyset \end{array}$$

$m = 1, m' = 0 : \sqrt{1(1+1) - 0(0+1)} = \sqrt{2}$

$m = 0, m' = -1 : \sqrt{1(1+1) - (-1)(-1+1)} = \sqrt{2}$

$$L_+ = \hbar\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad L_+\begin{pmatrix}0\\1\\0\end{pmatrix} = \sqrt{2}\hbar\begin{pmatrix}1\\0\\0\end{pmatrix} \qquad L_+\begin{pmatrix}1\\0\\0\end{pmatrix} = \emptyset \qquad \text{OK}$$

$$L_- = \hbar\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$$l = 2 \quad \begin{pmatrix} 0 & - & & \emptyset & \\ & 0 & - & & \\ & & 0 & - & \\ 0 & & & 0 & - \\ & & & & 0 \end{pmatrix}$$

$m = 2, m' = 1 : \sqrt{2(2+1) - 1(1+1)} = 2$

$m = 1, m' = 0 : \sqrt{2(2+1) - 0(0+1)} = \sqrt{6}$

$m = 0, m' = -1 : \quad \sqrt{6}$

$m = -1, m' = -2 : \sqrt{2(2+1) + 2(-2+1)} = 2$

$$L_+ = \hbar\begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ & 0 & \sqrt{6} & 0 & 0 \\ & & 0 & \sqrt{6} & 0 \\ & \emptyset & & 0 & 2 \\ & & & & 0 \end{pmatrix}$$

2022-UKM
-T8.2.

$L_+ : \sqrt{l(l+1) - m(m+1)}$

pokud $m = l \to \sqrt{l(l+1) - l(l+1)} = 0$

tedy $L_+ |l\ m=l\rangle = 0$

$L_+|1\,1\rangle = 0$ atp.

$L_\pm = L_x \pm i L_y \to L_+ = L_x + iL_y \to L_x = \frac{1}{2}(L_+ + L_-)$

$L_- = L_x - iL_y \qquad L_y = \frac{1}{2i}(L_+ - L_-)$

pro $l=1$

$\to L_x = \frac{\hbar}{2}\begin{pmatrix}0&\sqrt2&0\\ \sqrt2&0&\sqrt2\\ 0&\sqrt2&0\end{pmatrix} \qquad L_y = \frac{\hbar}{2i}\begin{pmatrix}0&\sqrt2&0\\ -\sqrt2&0&\sqrt2\\ 0&-\sqrt2&0\end{pmatrix}$

$L_z = \hbar\begin{pmatrix}1&&\\&0&\\&&-1\end{pmatrix} \qquad L_z^2 = \hbar^2\begin{pmatrix}1&&\\&0&\\&&1\end{pmatrix}$

$L_x^2 = \frac{\hbar^2}{4}\begin{pmatrix}2&0&2\\0&4&0\\2&0&2\end{pmatrix} = \hbar^2\begin{pmatrix}\frac12&0&\frac12\\0&1&0\\\frac12&0&\frac12\end{pmatrix} \qquad L_y^2 = \frac{\hbar^2}{4i^2}\begin{pmatrix}-2&0&2\\0&-4&0\\2&0&-2\end{pmatrix} = \hbar^2\begin{pmatrix}\frac12&0&-\frac12\\0&1&0\\-\frac12&0&\frac12\end{pmatrix}$

$L_x^2 + L_y^2 + L_z^2 = \hbar^2\begin{pmatrix}2&&0\\&2&\\0&&2\end{pmatrix}$ ok

$[L_i, L_j] = \varepsilon_{ijk}\, i\hbar L_k \qquad L_xL_y - L_yL_x \stackrel{?}{=} i\hbar L_z$

$L_xL_y = \frac{\hbar^2}{4i}\begin{pmatrix}-2&0&2\\0&0&0\\-2&0&2\end{pmatrix} \qquad L_yL_x = \frac{\hbar^2}{4i}\begin{pmatrix}2&0&2\\0&0&0\\-2&0&-2\end{pmatrix} \qquad L_xL_y - L_yL_x = \frac{\hbar^2}{4i}\begin{pmatrix}-4&0&0\\0&0&0\\0&0&4\end{pmatrix} = i\hbar^2\begin{pmatrix}1&&0\\&0&\\0&&-1\end{pmatrix}$

$= i\hbar L_z$ ■

$L_x^2 = \frac{1}{2}(L_+ + L_-)^2 = \frac{1}{4}(L_+^2 + L_-^2 + L_+L_- + L_-L_+)$

$L_y^2 = \frac{1}{2i}(L_+ - L_-)^2 = -\frac{1}{4}(L_+^2 + L_-^2 - L_+L_- - L_-L_+)$

$\Big\} \frac{1}{4}(2L_+L_- + 2L_-L_+)$

$= \frac{1}{2}(L_+L_- + L_-L_+)$

2022-UKM-T9.3

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$ $\quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$

$L^2 Y_0^0 = 0 \qquad L^2 Y_1^0 = \hbar^2 1(1+1) = 2\hbar^2$

$L_z Y_0^0 = 0 \qquad L_z Y_1^0 = 0$

$\psi = \frac{1}{\sqrt{2}}(Y_0^0 + Y_1^0) \qquad L^2\psi = \frac{1}{\sqrt{2}}(0\cdot Y_0^0 + 2\hbar^2 Y_1^0) = \sqrt{2}\hbar^2 Y_1^0 \neq \lambda\psi$ není vl. fce

$L_z\psi = \frac{1}{\sqrt{2}}(0\cdot Y_0^0 + 0\cdot Y_1^0) = 0\cdot\psi = \lambda\psi$ je vl. fce

$\langle\psi|L^2|\psi\rangle = \langle\psi|\sqrt{2}\hbar^2|Y_1^0\rangle = \frac{1}{\sqrt{2}}\sqrt{2}\hbar^2 = \boxed{\hbar^2} \qquad \langle L_z\rangle = 0$

$L_z Y_0^0 = -i\hbar\frac{\partial}{\partial\phi}\frac{1}{\sqrt{4\pi}} = 0 \qquad L_z Y_1^0 = -i\hbar\frac{\partial}{\partial\phi}\sqrt{\frac{3}{4\pi}}\cos\theta = 0$

$L^2 Y_0^0 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\frac{1}{\sqrt{4\pi}} = 0$

$L^2 Y_1^0 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \underbrace{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}}_{0}\right)\sqrt{\frac{3}{4\pi}}\cos\theta =$

$= -\hbar^2\sqrt{\frac{3}{4\pi}}\left(-\cos\theta + \frac{\cos\theta}{\cancel{\sin\theta}}(-\cancel{\sin\theta})\right) = -\hbar^2\sqrt{\frac{3}{4\pi}}(-2)\cos\theta$

$= 2\hbar^2\sqrt{\frac{3}{4\pi}}\cos\theta = 2\hbar^2 Y_1^0$

$\langle\psi|L^2|\psi\rangle \iint\frac{1}{2}\left(\frac{1}{\sqrt{4\pi}} + \sqrt{\frac{3}{4\pi}}\cos\theta\right)\left[-\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\left(\frac{1}{\sqrt{4\pi}} + \sqrt{\frac{3}{4\pi}}\cos\theta\right)$ $\quad d\theta\sin\theta\, d\phi$

$= -\frac{\hbar^2}{2}\int_0^{\pi}\int_0^{2\pi} d\theta\sin\theta\, d\phi\left(\frac{1}{\sqrt{4\pi}} + \sqrt{\frac{3}{4\pi}}\cos\theta\right)\cdot\sqrt{\frac{3}{4\pi}}(-2\cos\theta)$

$= \hbar^2\int_0^{\pi}\int_0^{2\pi} d\theta\sin\theta\,\underbrace{d\phi}_{2\pi}\left[\frac{\sqrt{3}}{4\pi}\cos\theta + \frac{3}{4\pi}\cos^2\theta\right] \qquad \cos\theta = t, \quad -\sin\theta\, d\theta = dt$

$= \frac{2\pi\hbar^2}{4\pi}\int_1^{-1}(-dt)\left[\sqrt{3}t + 3t^2\right] \rightarrow \int_{-1}^{1} dt$

$= \frac{\hbar^2}{2}\int_{-1}^{1}\left[\underbrace{\frac{\sqrt{3}t^2}{2}\Big|_{-1}^{1}}_{=0} + \frac{3t^3}{3}\Big|_{-1}^{1}\right] = \frac{\hbar^2}{2}\cdot 2 = \boxed{\hbar^2}$ OK

$L_z = \hbar\begin{pmatrix}0 & & & \\ & 1 & & 0\\ & & 0 & \\ 0 & & & -1\end{pmatrix} \qquad L^2 = \hbar^2\begin{pmatrix}0 & & & \\ & 2 & & 0\\ & & 2 & \\ 0 & & & 2\end{pmatrix} \qquad \psi = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix}$

$\langle L_z\rangle = \psi^T L_z\psi = \hbar\frac{1}{2}(1\;0\;1\;0)\begin{pmatrix}0 & & & \\ & 1 & & \\ & & 0 & \\ & & & -1\end{pmatrix}\begin{pmatrix}1\\0\\1\\0\end{pmatrix} = \frac{\hbar}{2}(1\;0\;1\;0)\begin{pmatrix}0\\0\\0\\0\end{pmatrix} = 0$

$\langle L^2\rangle = \psi^T L^2\psi = \hbar^2\frac{1}{2}(1\;0\;1\;0)\begin{pmatrix}0 & & & \\ & 2 & & \\ & & 2 & \\ & & & 2\end{pmatrix}\begin{pmatrix}1\\0\\1\\0\end{pmatrix} = \frac{\hbar^2}{2}(1\;0\;1\;0)\begin{pmatrix}0\\0\\2\\0\end{pmatrix} = \frac{2\hbar^2}{2} = \boxed{\hbar^2}$ OK

2022-UKM I10.1.

$L_+, L_-$ na stav $|lm\rangle$ v $\theta\phi$
mat. elementy $x,y,z \to$ CGC
komut. relace $[L_+, L_-]$ $[L_x, L_y]$ ? v $\theta\phi$ fix commutators

---

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta \qquad Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi}$$

$$L_x = i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \cos\phi \cotg\theta \frac{\partial}{\partial\phi}\right)$$

$$L_y = i\hbar\left(-\cos\phi \frac{\partial}{\partial\theta} + \sin\phi \cotg\theta \frac{\partial}{\partial\phi}\right)$$

$$L_z = -i\hbar \frac{\partial}{\partial\phi}$$

$$\cancel{L_x L_z = i(-i)\hbar^2 (\sin\phi \partial}$$

$$L_z Y_1^1 = -i\hbar \frac{\partial}{\partial\phi}\left(-\sqrt{\frac{3}{8\pi}}\right)\sin\theta\, e^{i\phi} = i\hbar\sqrt{\frac{3}{8\pi}}\, i \sin\theta\, e^{i\phi} = -\hbar\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi}$$

$$L_x Y_1^1 = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cos\phi \cotg\theta \frac{\partial}{\partial\phi}\right)\left(-\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}\right)$$

$$= -i\hbar\sqrt{\frac{3}{8\pi}}\left[\sin\phi\, e^{i\phi}\cos\theta + \cos\phi \frac{\cos\theta}{\sin\theta} \sin\theta\,(i)\, e^{i\phi}\right]$$

$$= -i\hbar\sqrt{\frac{3}{8\pi}}\left[\sin\phi\, e^{i\phi}\cos\theta + \cos\phi\cos\theta\, i\, e^{i\phi}\right]$$

$$= -i\hbar\sqrt{\frac{3}{8\pi}} \cos\theta\, e^{i\phi}\, i\,[\cos\phi - i\sin\phi] = -i\hbar\sqrt{\frac{3}{8\pi}}\cos\theta\, e^{i\phi}\, i\, e^{-i\phi} = \hbar\sqrt{\frac{3}{8\pi}}\cos\theta$$

přeslapíně? NE?

$$L_+ = L_x + iL_y = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cos\phi\cotg\theta\frac{\partial}{\partial\phi} - i\cos\phi\frac{\partial}{\partial\theta} + i\sin\phi\cotg\theta\frac{\partial}{\partial\phi}\right)$$

$$= i\hbar\left(-i\, e^{i\phi}\frac{\partial}{\partial\theta} + e^{i\phi}\cotg\theta\frac{\partial}{\partial\phi}\right)$$

$$= \hbar\left(e^{i\phi}\frac{\partial}{\partial\theta} + i e^{i\phi}\cotg\theta\frac{\partial}{\partial\phi}\right) = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cotg\theta\frac{\partial}{\partial\phi}\right)$$

$$\sin\phi - i\cos\phi = -i\cos\phi - i\left(\frac{1}{-i}\right)\sin\phi = -i(\cos\phi + i\sin\phi)$$

$$L_- = \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cotg\theta\frac{\partial}{\partial\phi}\right)$$

$$L_+ f(\theta,\phi) = \hbar e^{i\phi}\frac{\partial f}{\partial\theta} + i\hbar\cotg\theta\, e^{i\phi}\frac{\partial f}{\partial\phi} \qquad L_- f(\theta,\phi) = \hbar e^{-i\phi}\left(-\frac{\partial f}{\partial\theta} + i\cotg\theta\frac{\partial f}{\partial\phi}\right)$$

$$L_- L_+ f(\theta,\phi) = \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cotg\theta\frac{\partial}{\partial\phi}\right)\hbar e^{i\phi}\left(\frac{\partial f}{\partial\theta} + i\cotg\theta\frac{\partial f}{\partial\phi}\right)$$

$$= \hbar^2 e^{-i\phi}\left[e^{i\phi}\left(-\frac{\partial^2 f}{\partial\theta^2}\right) + i\frac{\partial}{\partial\phi} \ldots \ldots\right.$$

$$[L_+, L_-] = [L_x + iL_y, L_x - iL_y] = -i[L_x, L_y] + i[L_y, L_x] = -2i\hbar L_z$$

2022-UKM-TMO2

$\langle Y_0^0 | x | Y_{l'}^{m'} \rangle = ?$

$x = \boxed{r} \sin\theta\cos\phi$
$y = \boxed{r} \sin\theta \sin\phi$
$z = \boxed{r} \cos\theta$
elsewhere

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$

$Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$

$Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$

$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$

$Y_0^0 \cdot x(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \cdot \sin\theta\cos\phi$

$= \frac{1}{\sqrt{4\pi}} \sin\theta \frac{1}{2}(e^{i\phi} + e^{-i\phi})$

$= \frac{1}{\sqrt{16\pi}} \sin\theta e^{i\phi} + \frac{1}{\sqrt{16\pi}} \sin\theta e^{-i\phi}$

$= -\sqrt{\frac{1}{6}}\left(-\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}\right)$
$+ \sqrt{\frac{1}{6}}\left(\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}\right)$

$\langle Y_0^0 | \sin\theta\cos\phi | Y_1^1 \rangle$

$= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{1}{\sqrt{4\pi}} \sin\theta \underbrace{\cos\phi}_{\frac{1}{2}(e^{i\phi}+e^{-i\phi})} \left(-\sqrt{\frac{3}{8\pi}}\right) \sin\theta\, e^{i\phi}$

$(1-\cos^2\theta)\sin\theta$

$= \frac{1}{2}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \left(-\frac{\sqrt{3}}{4\pi\sqrt{2}}\right) \sin^3\theta = -\frac{\sqrt{3}}{8\pi\sqrt{2}} 2\pi \int_0^{\pi} d\theta \sin^3\theta$

$t = \cos\theta$
$dt = -\sin\theta\, d\theta$

$= -\frac{\sqrt{3}}{4\sqrt{2}} \int_{1}^{-1} (1-t^2)(-dt)$

$= -\frac{\sqrt{3}}{4\sqrt{2}} \left[ t\Big|_{-1}^{1} - \frac{t^3}{3}\Big|_{-1}^{1} \right] = -\frac{\sqrt{3}}{4\sqrt{2}}\left[2 - \frac{2}{3}\right] = -\frac{\sqrt{3}}{4\sqrt{2}} \cdot \frac{4}{3} = -\frac{1}{\sqrt{6}}$

$\langle Y_0^0 | \cos\theta | Y_1^0 \rangle = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{1}{\sqrt{4\pi}} \cos\theta \sqrt{\frac{3}{4\pi}} \cos\theta$

$= \frac{2\pi}{4\pi} \cdot \sqrt{3} \int_0^{\pi} \cos^2\theta \sin\theta\, d\theta = \frac{\sqrt{3}}{2} \int_{-1}^{1} t^2 dt = \frac{\sqrt{3}}{2} \frac{t^3}{3}\Big|_{-1}^{1} = \frac{\sqrt{3}}{2} \cdot \frac{2}{3} = \frac{1}{\sqrt{3}}$

$\frac{1}{\sqrt{4\pi}} \cdot \cos\theta = \frac{1}{\sqrt{3}} \cdot \sqrt{\frac{3}{4\pi}} \cdot \cos\theta = \frac{1}{\sqrt{3}} Y_1^0$

$\langle Y_1^0 | \cos\theta | Y_2^0 \rangle = \iint \sqrt{\frac{3}{4\pi}} \cos\theta \cos\theta \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) \sin\theta d\theta d\phi$

$= \frac{2\pi}{8\pi} \sqrt{15} \int_0^{\pi} d\theta \sin\theta \cos^2\theta (3\cos^2\theta - 1)$

$= \frac{\sqrt{15}}{4} \int_{-1}^{1} t^2(3t^2-1) dt = \frac{\sqrt{15}}{4}\left[\frac{3t^5}{5}\Big|_{-1}^{1} - \frac{t^3}{3}\Big|_{-1}^{1}\right] = \frac{\sqrt{15}}{4}\left[\frac{6}{5} - \frac{2}{3}\right] =$

$= \frac{\sqrt{15}}{4}\left(\frac{18}{15} - \frac{10}{15}\right) = \frac{2}{\sqrt{15}}$ fair enough

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$\left[\frac{\partial}{\partial\phi}, \frac{\partial}{\partial\theta}\right] = 0$ (platí ne)

$\frac{\partial}{\partial\phi}\frac{\partial}{\partial\theta}\sin\theta e^{i\phi} = i\cos\theta e^{i\phi}$, nezáleží na pořadí

$\left[\sin\theta\frac{\partial}{\partial\phi}, \frac{\partial}{\partial\theta}\right] = \cancel{\alpha}..$ to u zásí ne

$\sin\theta\frac{\partial}{\partial\phi}\frac{\partial}{\partial\theta} f(\theta,\phi) = \sin\theta\ \frac{\partial^2 f(\theta,\phi)}{\partial\phi\partial\theta}$

$\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\phi} f(\theta,\phi) = \frac{\partial}{\partial\theta}\ \sin\theta\ \frac{\partial f}{\partial\phi} = \cos\theta\frac{\partial f}{\partial\phi} + \sin\theta\frac{\partial^2 f}{\partial\theta\partial\phi}$

$\left[\sin\theta\frac{\partial}{\partial\phi}, \frac{\partial}{\partial\theta}\right] f = \sin\theta\ \frac{\partial^2 f}{\partial\theta\partial\phi} - \cos\theta\frac{\partial f}{\partial\phi} - \sin\theta\frac{\partial^2 f}{\partial\phi\partial\theta} = -\cos\theta\frac{\partial f}{\partial\phi}$

$f = \sin\theta e^{i\phi}$

$\sin\theta\frac{\partial}{\partial\phi}\frac{\partial}{\partial\theta}\sin\theta e^{i\phi} = \sin\theta\ i\ e^{i\phi}\cos\theta$

$\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\phi}\sin\theta e^{i\phi} = i e^{i\phi}\, 2\cos\theta\cos\theta$

$[\quad]\sin\theta e^{i\phi} = -i e^{i\phi}\cos\theta\sin\theta = -\cos\theta\frac{\partial}{\partial\phi}(\sin\theta e^{i\phi})$ OK

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

vl. stavy $S_x$: $\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = +\lambda^2 - \frac{\hbar^2}{4} = (\lambda - \frac{\hbar}{2})(\lambda + \frac{\hbar}{2})$ $\left\langle \begin{matrix} \frac{\hbar}{2} \\ -\frac{\hbar}{2} \end{matrix} \right.$

$\begin{pmatrix} -\frac{\hbar}{2} & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\frac{\hbar}{2} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0 \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ pro $\lambda = \frac{\hbar}{2}$ $\quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ pro $\lambda = -\frac{\hbar}{2}$ , $\hat{A} = \sum_i a_i |i\rangle\langle i|$

$\hat{S}_x = \sum_{s_x} s_x |s_x\rangle\langle s_x| = \frac{\hbar}{2} \frac{1}{\sqrt{2}}(1 \; 1) \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{\hbar}{2}\frac{1}{2}(1 \; -1)\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$= \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{\hbar}{4}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \cancel{\frac{\hbar}{4}\begin{pmatrix} 0 & 2 \\ 0 & 2 \end{pmatrix}} = \frac{\hbar}{4}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

OK

$s_x^+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $s_x^- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ ← vl. stavy vyjádřené v bázi $s_z$

$s_x^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $s_x^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ← vl. stavy vyjádřené v bázi $s_x$

$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

$S_z$ v bázi $s_x$

$U^+ S_z U^+ = \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \frac{\hbar}{4}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

OK

- spin z minule
- mat. element vodík
- gauss pro H?
- čas závislost! ⟨ ⟩ ωt! DU - Ehrenfest



H - atom

$R_{nl}$ : $R_{10} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$ $\qquad R_{20} = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/(2a_0)}$

(r-ová) $R_{21} = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/(2a_0)}$ $\qquad R_{31} = \frac{4}{81\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6 - \frac{Zr}{a_0}\right)\frac{Zr}{a_0} e^{-Zr/(3a_0)}$

$Y_0^0 = \frac{1}{\sqrt{4\pi}} \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta \qquad Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}$

· normalizace $R_{nl}$ : $Z = 1$ ← vodík $\qquad \int [uv]' = \int u'v + \int uv'$

$$\int_0^\infty r^2 dr\, 4\left(\frac{1}{a_0^3}\right) e^{-2r/a_0} \underset{p.p.}{=} \frac{4}{a_0^3}\left[r^2 \frac{a_0}{2}(-1) e^{-2r/a_0}\right]_0^\infty - \frac{4}{a_0^3}\int_0^\infty 2r \frac{a_0}{2}(-1) e^{-2r/a_0} dr$$

$$= \frac{4}{a_0^2}\int_0^\infty r e^{-2r/a_0} dr = \frac{4}{a_0^2}\left[r\left(-\frac{a_0}{2}\right) e^{-2r/a_0}\right]_0^\infty - \frac{4}{a_0^2}\int_0^\infty \left(-\frac{a_0}{2}\right) e^{-2r/a_0} dr$$

$$= \frac{2}{a_0}\int_0^\infty e^{-2r/a_0} dr = \frac{2}{a_0}\left(-\frac{a_0}{2}\right) e^{-2r/a_0}\Big|_0^\infty = -[0 - 1] = \underline{1}$$

$$\int_0^\infty r^n e^{-\alpha r} dr = \underbrace{\left[r^n\left(-\frac{1}{\alpha}\right) e^{-\alpha r}\right]_0^\infty}_{\to 0} + \int_0^\infty \frac{n}{\alpha} r^{n-1} e^{-\alpha r} dr \dots \frac{n!}{\alpha^n}\int_0^\infty e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}}$$

$x = r\sin\theta\cos\phi \quad \rightsquigarrow \quad r\sin\theta e^{i\phi}$

$$\langle R_{10} Y_{00} | r \underset{\text{jako } (Y_1^{-1})^*}{\sin\theta e^{i\phi}} | R_{21} Y_1^{-1}\rangle = \langle R_{10}|r|R_{21}\rangle \langle Y_{00}|\sin\theta e^{i\phi}| Y_1^{-1}\rangle$$

$$\langle R_{10}|r|R_{21}\rangle = \frac{2}{a_0^{3/2}} \frac{1}{2\sqrt{6}} \frac{1}{a_0^{3/2}} \int_0^\infty e^{-r/a_0} \frac{r}{a_0} e^{-r/(2a_0)} r^2 dr$$

$$= \frac{1}{a_0^4\sqrt{6}}\int_0^\infty r^3 e^{-\frac{3r}{2a_0}} dr = \frac{1}{a_0^4\sqrt{6}} \frac{3!}{\left(\frac{3}{2a_0}\right)^4} = \frac{6\, \cancel{a_0^4}\, 2^4}{\cancel{a_0^4}\, 3^4 \sqrt{6}} = \frac{\sqrt{6}\cdot 16}{81}$$

$$\langle Y_{00}|\sin\theta e^{i\phi}|Y_1^{-1}\rangle = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{8\pi}} \sin\theta \cancel{e^{-i\phi}} \sin\theta \cancel{e^{i\phi}}$$

$$= \frac{2\pi\sqrt{3}}{4\pi\sqrt{2}}\int_0^\pi \sin^3\theta\, d\theta = \frac{1}{2}\sqrt{\frac{3}{2}}\int_{-1}^1 (1 - t^2) dt = \frac{1}{2}\sqrt{\frac{3}{2}}\underbrace{\left[t - \frac{t^3}{3}\right]_{-1}^1}_{2 - \frac{2}{3}} = \frac{1}{2}\sqrt{\frac{3}{2}}\frac{4}{3} = \frac{\sqrt{2}}{\sqrt{3}}$$

$$\langle R_{10}|r|R_{31}\rangle = 2\cdot\frac{4}{81\sqrt{6}}\frac{1}{a_0^3}\int_0^\infty r^2 dr\left(6 - \frac{r}{a_0}\right)\frac{r}{a_0} e^{-r/a_0} e^{-r/3a_0}$$

$$= \frac{8}{81\sqrt{6}}\frac{1}{a_0^3}\int_0^\infty r^2 dr\left[6\frac{r^3}{a_0} - \frac{r^4}{a_0^2}\right] e^{-\frac{4r}{3a_0}}$$

$$= \frac{8}{81\sqrt{6}}\frac{1}{a_0^3}\left(6\cdot\frac{3!}{a_0}\left(\frac{3a_0}{4}\right)^4 - \frac{4!}{a_0^2}\cdot\left(\frac{3a_0}{4}\right)^5\right) = \frac{8}{81\sqrt{6}}\left(6\cdot 36\cdot\frac{81}{256} - 24\cdot\frac{243}{512}\right)$$

$$= \frac{1}{\sqrt{6}}\left(36\cdot\frac{1}{32} - \frac{3\cdot 24}{64}\right) = \frac{1}{\sqrt{6}}\left(\frac{9}{8} - \frac{9}{8}\right) = 0\ ?$$

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$$\langle R_{10}|r|R_{31}\rangle = 2\cdot\frac{4}{81\sqrt{6}}\frac{1}{a_0^3}\int_0^\infty r^3 dr\left(\frac{6r}{a_0}-\frac{r^2}{a_0^2}\right)e^{-4r/3a_0}$$

$$= \frac{8}{81\sqrt{6}}\frac{1}{a_0^3}\int_0^\infty\left(\frac{6r^4}{a_0}-\frac{r^5}{a_0^2}\right)e^{-\frac{4r}{3a_0}}dr$$

$$= \frac{8}{81\sqrt{6}}\frac{1}{a_0^3}\left[6\cdot\frac{4!}{a_0}\cdot\left(\frac{3a_0}{4}\right)^5-\frac{5!}{a_0^2}\left(\frac{3a_0}{4}\right)^6\right]$$

$$= \frac{8a_0}{81\sqrt{6}}\left[\frac{6\cdot 4!\,3^5}{4^5}-\frac{5!\,3^6}{4^6}\right]$$

$$= a_0\cdot\left[\frac{3\cdot 9\cdot 6\cdot 2\cdot 3!}{4^3}-\frac{2\cdot 27\cdot 2\cdot 5\cdot 3!}{4^4}\right]$$

$$= a_0\left[\frac{9\cdot 9\cdot 2}{16}-\frac{27\cdot 5\cdot 3}{64}\right] = a_0\left[\frac{81\cdot 8-81\cdot 5}{64}\right]$$

$$= \frac{a_0\, 81\cdot 3}{64} = a_0\left(\frac{3^5}{4^3}\right) \text{ (qui) } \neq 0$$

$\psi = N\exp(-\alpha r^2)$ 2022-clear-TM3

$$\langle\psi|\psi\rangle = N^2 \underbrace{\int_0^{2\pi} d\phi \int_0^{\pi} d\Theta \sin\Theta}_{4\pi} \int_0^{\infty} r^2 dr\, e^{-2\alpha r^2}$$

$$= 4\pi N^2 \cdot \underbrace{\int_0^{\infty} r^2 e^{-2\alpha r^2} dr}$$

$$= \frac{1}{2}\int_{-\infty}^{\infty} r^2 e^{-\underbrace{2\alpha}_{A=2\alpha} r^2} dr \qquad \frac{1}{2A}\sqrt{\frac{\pi}{A}} = \frac{1}{4\alpha}\sqrt{\frac{\pi}{2\alpha}}$$

$$= \frac{1}{8\alpha}\sqrt{\frac{\pi}{2\alpha}}$$

$$1 = 4\pi N^2 \frac{1}{8\alpha}\sqrt{\frac{\pi}{2\alpha}} = \frac{\pi N^2}{2\alpha}\sqrt{\frac{\pi}{2\alpha}} = 1$$

$$N^2 = \sqrt{\frac{\alpha}{\pi}}\ \frac{2\alpha}{\pi}$$

$$N = \sqrt[4]{\frac{\alpha}{\pi}}\sqrt{\frac{2\alpha}{\pi}} = \left(\frac{2\alpha}{\pi}\right)^{3/4} \quad \text{ok}$$

$$T|\psi\rangle = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} N e^{-\alpha r^2}$$

$$= -\frac{\hbar^2 N}{2m}\frac{1}{r^2}\frac{d}{dr} r^2(-\alpha)2r\, e^{-\alpha r^2}$$

$$= \frac{2\hbar^2 N\alpha}{2m}\frac{1}{r^2}\frac{d}{dr} r^3 e^{-\alpha r^2}$$

$$= \frac{N\alpha\hbar^2}{m}\frac{1}{r^2}\left(3r^2 e^{-\alpha r^2} - \alpha r^3 e^{-\alpha r^2} 2r\right)$$

$$= \frac{N\alpha\hbar^2}{m}\left[3e^{-\alpha r^2} - 2r^2\alpha e^{-\alpha r^2}\right]$$