# QMI - 5 | částice ve 3D – odbočka Q-teorie momentu hybnosti

## OPAKOVÁNÍ

**Def**: operátor <u>momentu hybnosti</u> $\hat{\vec{J}} \equiv (\hat J_1, \hat J_2, \hat J_3)$

pokud splňuje $[\hat J_\alpha, \hat J_\beta] = i\hbar\, \varepsilon_{\alpha\beta\gamma} \hat J_\gamma$

**Důsledky**: $[\hat J^2, \hat J_\alpha] = 0 \quad \forall \alpha = 1,2,3$    $x, y, z$

např. společná báze $\hat J^2, J_3$ : $\hat J^2 |jm\rangle = \hbar^2 j(j+1) |jm\rangle$

$J_3 |jm\rangle = \hbar\, m\, |jm\rangle$

kde $j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots\}$ a $\forall j$ : $m = \underbrace{-j, -j+1, \dots, j-1, j}_{2j+1 \text{ hodnot}}$

Posunovací operátory : $\hat J_\pm \equiv \hat J_1 \pm i \hat J_2$

$[\hat J_\pm, \hat J^2] = 0$ (nemění hodnotu $j$)    $[\hat J_3, \hat J_\pm] = \pm\hbar J_\pm$

(posouvá $m$ o $\pm 1$)

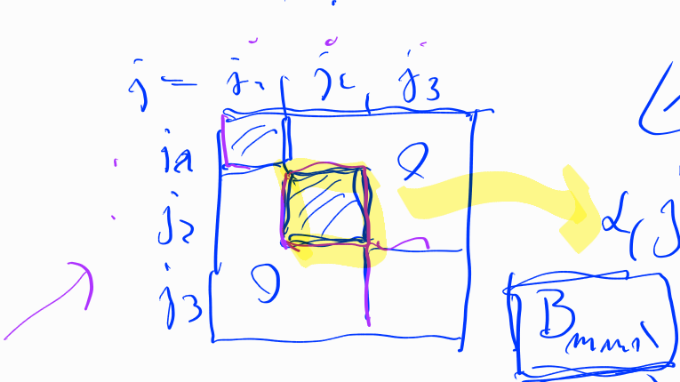
neboli $\hat J_\pm |jm\rangle = \hbar \sqrt{(j \mp m)(j \pm m + 1)}\, |j\, m \pm 1\rangle$

---

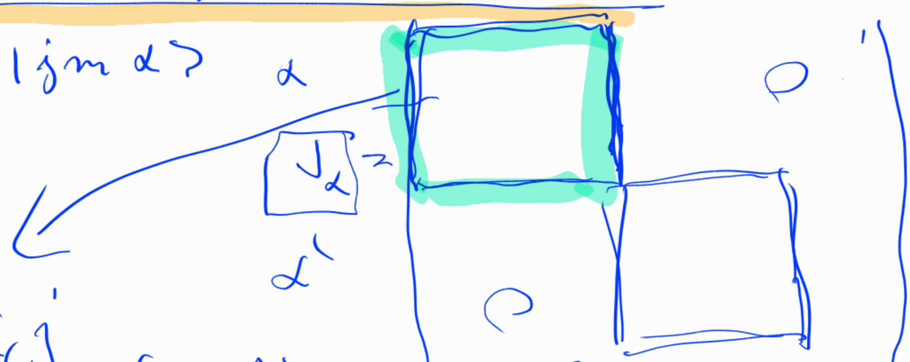
Př. mom. hybn. ... $\vec S = \frac{\hbar}{2}(\hat\sigma_1, \hat\sigma_2, \hat\sigma_3)$ ... $\hat{\vec L} = \hat{\vec x} \times \hat{\vec p}$

- Maticová reprezentace $\hat J_1, \hat J_2, \hat J_3$ na vl. podpr. $\hat J^2$

ÚSKO ... $\hat J^2, J_3, \hat A$ ... $|jm\alpha\rangle$




$\boxed{B_{mm'}}$




$[J_\alpha, \hat A] = 0$

$[J_\alpha, \hat J] = 0$

$[J_\alpha, J_3] \neq 0$

$J^2 = \sum_\alpha J_\alpha^2$

$J$    $j = \frac{1}{2}$    $\mathcal{H} = \mathbb{C}^2$

$$\boxed{\begin{aligned}\langle j m \alpha | J^2 | \alpha' j' m' \rangle &= \delta_{\alpha\alpha'}\, \delta_{jj'}\, \delta_{mm'} \cdot \hbar^2 j(j+1)\\ \langle j m \alpha | J_3 | \alpha' j' m' \rangle &= \delta_{\alpha\alpha'}\, \delta_{jj'}\, \delta_{mm'} \cdot \hbar m\\ \langle j m \alpha | J_\beta | \alpha' j' m' \rangle &= \delta_{\alpha\alpha'}\, \delta_{jj'}\, (J_\beta)^{(j)}_{mm'}\end{aligned}}$$

matice $n = (2j+1)\times(2j+1)$

$\beta = 1,2$

$\Rightarrow \quad J_\pm = J_1 \pm i J_2 \quad \to \quad \boxed{J_1 = \frac{1}{2}(J_+ + J_-)} \quad J_2 = \frac{1}{2i}(J_+ - J_-)$

$$\langle j m \alpha | J_+ | j' m' \alpha' \rangle = \delta_{\alpha\alpha'}\, \delta_{jj'}\, \delta_{m, m'+1}\, \hbar \sqrt{j'(j'+1) - m'(m'+1)}$$

$m$: $j, \dots, -j$

$J_- = (J_+)^\dagger$

$= J_- = \sqrt{(j-m)(j+m+1)}$

$\boxed{2j+1}$ $\quad (-) \sqrt{1 \cdot \boxed{2j}}$ $\quad \sqrt{2(2j-1)}$, $\; 3(2j-2)$

$\frac{1}{2} \colon -\frac{1}{2}$

| | $j = 0$ | spin 1/2 $\left(j = \frac{1}{2}\right)$ | spin 1 $j = 1$ | $j = \frac{3}{2}$ $\quad \frac{1\cdot 3}{2\;\;2}$ |
|---|---|---|---|---|
| $\hat{J}_+$ | $0$ | $\hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}\hbar$ | $\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}\hbar$ |
| $\hat{J}_1 = \hat{J}_x$ | $0$ | $\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_x$ | $\frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ | $\frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & & \\ \sqrt{3} & 0 & \sqrt{4} & \\ & \sqrt{4} & 0 & \sqrt{3} \\ & & \sqrt{3} & 0 \end{pmatrix}$ $\quad \sqrt{1\cdot 2j}$, $\sqrt{2\cdot 2j-1}$, $\vdots$ |
| $\hat{J}_2$ | $0$ | $\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ | $\frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$ | $\frac{\hbar}{2}\begin{pmatrix} 0 & -\sqrt{3}i & & \\ \sqrt{3}i & 0 & -2i & \\ & 2i & 0 & -\sqrt{3}i \\ & & \sqrt{3}i & 0 \end{pmatrix}$ |
| $J_z$ | $0$ | $\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ | $\hbar\begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}$ | $\frac{\hbar}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$ |

OK $\qquad \hbar\, \delta_{mm'} \cdot m$

$\to$ částice se spinem $j$ ... $\boxed{\hat{J}_\alpha}$ operátory matice $(2j+1)\times(2j+1)$ $\quad \mathcal{H} = \mathbb{C}^{2j+1}$

# OPERÁTOR L v x-reprezentaci a jeho vl. v. a vl. č.

$\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}} = \hat{\vec{x}} \times (-i\hbar \vec{\nabla}_x)$ je samosdruž.

$\hat{L}_x = -i\hbar (y\partial_z - z\partial_y)$

$L_y = -i\hbar (z\partial_x - x\partial_z)$

$L_z = -i\hbar (x\partial_y - y\partial_x)$

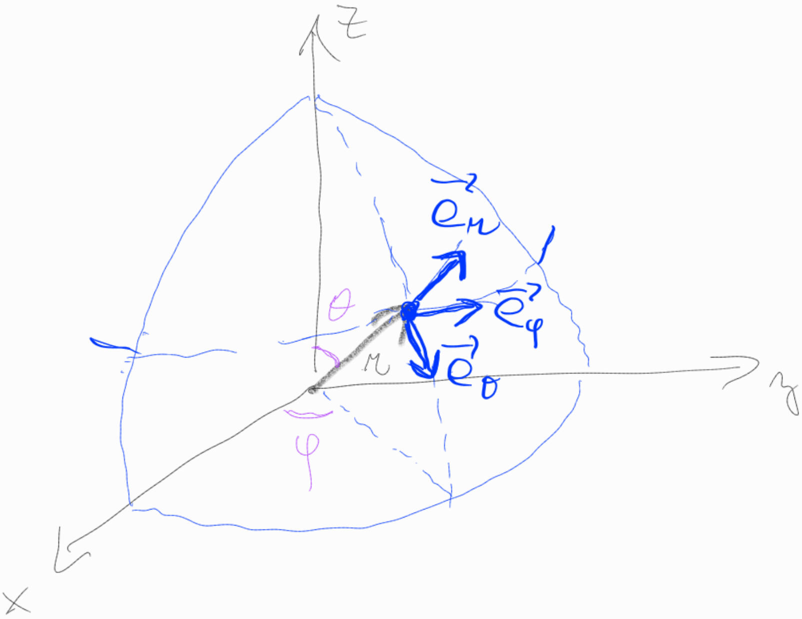
$[L_\alpha, L_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} L_\gamma$

pozn. p-reprezentace

$\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}} = i\hbar \vec{\nabla}_p \times \vec{p} = \vec{p} \times (-i\hbar \vec{\nabla}_p)$

$\hat{L}^2, \hat{L}_z \;\dots\; |lm\rangle \dots \psi_{lm}(\vec{x})$

# Sférické souřadnice




Lamé

$x = r\cos\varphi \sin\theta$ $\quad h_r = 1$

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

$z = r\cos\theta$ $\quad h_\varphi = r\sin\theta$

metrické koef. v OG souř.

$ds^2 = h_r^2 dr^2 + h_\theta^2 d\theta^2 + h_\varphi^2 d\varphi^2$

$\vec{e}_r = \frac{\partial}{\partial r}(x,y,z) = \cos\varphi \sin\theta \cdot \vec{e}_x + \sin\varphi \sin\theta \cdot \vec{e}_y + \cos\theta \vec{e}_z$

$\vec{e}_\theta = \frac{1}{h_\theta}\frac{\partial}{\partial\theta}(x,y,z) = \cos\varphi\cos\theta \, \vec{e}_x + \sin\varphi\cos\theta \, \vec{e}_y - \sin\theta \vec{e}_z$

$\vec{e}_\varphi = \frac{1}{h_\varphi}\frac{\partial}{\partial\varphi}(x,y,z) = -\sin\varphi \vec{e}_x + \cos\varphi \vec{e}_y$

$$\begin{pmatrix} \vec{e}_r \\ \vec{e}_\theta \\ \vec{e}_\varphi \end{pmatrix} = M \begin{pmatrix} \vec{e}_x \\ \vec{e}_y \\ \vec{e}_z \end{pmatrix}$$

-- M je OG matice $M^{-1} = M^T$

operátor $\vec{L} = -i\hbar \hat{\vec{x}} \times \vec{\nabla} = -i\hbar (r\vec{e}_r) \times \left( \vec{e}_r \frac{\partial}{\partial r} + \frac{\vec{e}_\theta}{h_\theta}\frac{\partial}{\partial\theta} + \frac{\vec{e}_\varphi}{h_\varphi}\frac{\partial}{\partial\varphi} \right)$

$\vec{e}_r \times \vec{e}_r = 0 \qquad \vec{e}_r \times \vec{e}_\theta = +e_\varphi \qquad \vec{e}_r \times \vec{e}_\varphi = -\vec{e}_\theta$

$\Rightarrow$

$$\boxed{\vec{L} = -i\hbar\left(\vec{e}_\varphi \frac{\partial}{\partial\theta} - \frac{\vec{e}_\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)} = -i\hbar\begin{pmatrix} -\sin\varphi \frac{\partial}{\partial\theta} - \cos\varphi \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi} \\ \cos\varphi\frac{\partial}{\partial\theta} - \sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi} \\ \frac{\partial}{\partial\varphi}\end{pmatrix} = \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix}$$

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

-- $\hat{L}_\pm = L_x \pm i L_y = \hbar e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$

-- $\mathcal{H} \equiv L^2(\mathbb{R}^3) = \mathcal{H}_r \otimes \mathcal{H}_{S_2}$ -- $L_\alpha = \hat{I}_r \otimes \hat{L}_\alpha$

$|lm\rangle \in \mathcal{H}_{S_2}$ $\qquad |lm\alpha\rangle \equiv |\alpha\rangle \otimes |lm\rangle$

tj. $\langle\vec{x}|lm\rangle \leftrightarrow \boxed{Y_{lm}(\theta,\varphi)} \equiv \langle\vec{x}|lm\rangle$

$\qquad \cancel{r}, \theta, \varphi$

$\hat{L}^2 Y_{lm}(\theta,\varphi) = \hbar^2 l(l+1) Y_{lm}(\theta,\varphi)$

$\hat{L}_z Y_{lm}(\theta,\varphi) = \hbar m Y_{lm}(\theta,\varphi)$ — $-i\hbar\frac{\partial}{\partial\varphi}$

$\hookrightarrow \quad -i\partial_\varphi Y_{lm}(\theta,\varphi) = m Y_{lm}(\theta,\varphi)$ ..


$-i\partial_\varphi f(\varphi) = m f(\varphi) \longrightarrow$ spojitost v okli $\varphi = 0, 2\pi$

$\quad \hookrightarrow \underline{e^{im\varphi}}$ . $1 = e^{im0} = e^{im2\pi} \ldots e^{2\pi i m} = 1$

$\qquad m \in \mathbb{Z}$

$\Rightarrow l \in \mathbb{Z}$ $\qquad m = -l, -l+1, \ldots$

vidimo, da $\sigma_{L^2}$ .. je dano $l = 0, 1, 2, 3, \ldots$

$\sigma_{L^2} \equiv \{\hbar l(l+1),\ l \in \mathbb{Z}_0^+\}$ $\mathbb{N}_0$

---

$\hat{L}^2$ ? $\quad L^2 = -\hbar^2\left[\vec{e}_\varphi\frac{\partial}{\partial\theta} - \frac{\vec{e}_\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right]\left[\vec{e}_\varphi\frac{\partial}{\partial\theta} - \frac{\vec{e}_\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right]$

$\vec{e}_\varphi \quad \vec{e}_\theta \qquad \frac{\partial}{\partial\theta}\vec{e}_\varphi = 0 \qquad \frac{\partial \vec{e}_\varphi}{\partial\varphi} = -(\cos\varphi, \sin\varphi, 0)^T = -\vec{e}_r\sin\theta$

$\qquad -\vec{e}_\theta\cos\theta$

$\frac{\partial\vec{e}_\theta}{\partial\theta} = -\vec{e}_r \qquad \frac{\partial\vec{e}_\theta}{\partial\varphi} = \cos\theta\,\vec{e}_\varphi$

$$\hat{L}^2 = -\hbar^2 \left[ \frac{\partial^2}{\partial\vartheta^2} + \frac{\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \right]$$

srovn.: $\Delta$ - operátor ve sféř. souř.

$$\Delta = \frac{1}{h_r h_\theta h_\varphi}\left[ \frac{\partial}{\partial r}\frac{h_\theta h_\varphi}{h_r}\frac{\partial}{\partial r} + \frac{\partial}{\partial\theta}\frac{h_r h_\varphi}{h_\theta}\frac{\partial}{\partial\theta} + \frac{\partial}{\partial\varphi}\frac{h_r h_\theta}{h_\varphi}\frac{\partial}{\partial\varphi}\right]$$

$$= \frac{1}{r^2}\partial_r r^2 \partial_r + \frac{1}{r^2}\left\{ \underbrace{\frac{1}{\sin\theta}\partial_\theta \sin\theta \cdot \partial_\theta}_{\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\partial_\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

$$\boxed{\Delta = \mathrm{rad} - \frac{\hat{L}^2}{\hbar^2 r^2}}$$

$L^2$ úzce souvisí s $\Delta$

$$L^2 = -\hbar^2\left( r^2\Delta - \frac{\partial^2}{\partial r^2} - 2r\frac{\partial}{\partial r}\right)$$

? $Y_{lm}(\theta,\varphi)$

dále:

vlastní podprostory $L^2$, $L_z$

jsou homogenní polynomy $x, y, z$ stupně $l$; s podm.

$\boxed{\Delta p_l(x,y,z) = 0}$

$1, x, x^2, x^3, \dots$

- def homog. poly. st $l$ ... $p_l(x,y,z)$

$xy, yz, xz, \boxed{x^2 y}$

$1, y, y^2, y^3, \dots$

$1, z, z^2, z^2 \dots$

$p_l(x,y,z)$ .. $\mathcal{L}(x^a y^b z^c)$

$l = \mathrm{st}\, p = \max\{a+b+c\}$

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

... $\hookrightarrow$ $\mathcal{L}(x^a y^b z^c)$ ... $a+b+c = l$

$x^2, y^2, z^2, xy, xz, yz$

1) $p_e(x,y,z) = \underbrace{r^l}_{\text{sfer}} \underline{f(\theta,\varphi)}$

$r\cos\varphi\sin\theta$

2) $\underbrace{\hat{L}_\alpha p_e(x,y,z)}_{\text{pr}_1} = \tilde{p}_e(x,y,z)$

$\underline{L_z}$ $\quad x\partial_y \quad \underline{y\partial_x}$

$a+1 \quad b \to b-1 \quad l = a+b+c$ nezmění

3) $\Delta p_e(x,y,z) = \Delta_r r^l f(\theta,\varphi)$

$= \underline{f(\theta,\varphi)} \underbrace{\frac{1}{r^2}\partial_r r^2 \partial_r r^l}_{l r^{l+1}} - \frac{L^2}{\hbar^2} r^{l-2} f(\theta,\varphi)$

$l(l+1) r^{l-2}$

$= f(\theta,\varphi)\, l(l+1) \cancel{r^{l-2}} - \frac{\hat{L}^2}{\hbar^2} \cancel{r^{l-2}} f(\theta,\varphi) = 0 \quad / \hbar^2$

$\boxed{\hat{L}^2 f(\theta,\varphi) = \hbar^2 l(l+1) f(\theta,\varphi)}$ ... vl. fce $L^2$ ... $|lm\rangle$

vl. podpr. $L^2$ ... $l$ $\equiv$ homog $p_e(x,y,z)$ st $l$

$\Delta p_e = 0$

dim? $|lm\rangle$ $\underline{m = -l, -l+1 \dots l \; \dots \; 2l+1}$

dim $= 2l+1$

počet $p_e(x,y,z)$ $\Delta p = 0$

$\mathcal{L}(x^a y^b z^c)$ $\quad \underline{a+b+c} = l$ $\quad \dots N_e = (l+1) + l + l-1 \dots + 1$

$\underbrace{||\bullet \; \bullet \; \bullet|}_{a,\, b} \underbrace{\bullet \; \bullet \; \bullet||}_{c}$ $\quad = \frac{(l+2)(l+1)}{2}$

$l+1$ možn.

počet $p_\ell(x,y,z) = N_\ell = \frac{(\ell+2)(\ell+1)}{2}$ st. vol.

$\boxed{\Delta p_\ell = 0}$ ? $\quad \Delta p_\ell = \tilde{p}_{\ell-2} \equiv 0 \quad \ldots \underline{N_{\ell-2} = \frac{\ell(\ell-1)}{2}}$

$\dim \{ \forall p_\ell \text{ homog st } \ell;\ \Delta p_\ell = 0 \} = N_\ell - N_{\ell-2}$

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

---

vl. podpr $L^2$ .. vl. č. $\ell$ $= \{ p_\ell \text{ homog st } \ell,\ \Delta p_\ell = 0 \}$

$\Rightarrow \quad Y_{\ell m}(\theta, \varphi)$