QM II – 4 Tenzorové operátory. Ireducibilní složky, W-Eck.

OPAKOVÁNÍ

- grupa rotací SO(3) ... $R_{\vec{n}}(\alpha)$ / $R(\alpha,\beta,\gamma)$
- reprezentace $\mathcal{R}(R) = e^{-\frac{i}{\hbar}\alpha \hat{J}_z} e^{-\frac{i}{\hbar}\beta \hat{J}_y} e^{-\frac{i}{\hbar}\gamma \hat{J}_z}$ ... operátor na $\mathcal{H}$
- $\forall$ reprezentace $\exists U$: $U^{+}\mathcal{R}U = \begin{pmatrix} D^{(j_1)}_{mm'} & 0 & 0 \\ 0 & D^{(j_2)}_{mm'} & 0 \\ 0 & 0 & \ddots \end{pmatrix}$ IRR, IRR } Reducibilní reprezent.
- Vektorový operátor: def: $\hat{\mathcal{R}}^{+}(R)\hat{V}_k\hat{\mathcal{R}}(R) = \sum_l R_{kl}\hat{V}_l \quad \forall R$

$$\Longleftrightarrow \quad \boxed{[\hat{J}_k, \hat{V}_l] = i\hbar\,\varepsilon_{klm}\hat{V}_m}$$

- Zobecnění na tenzory: $\hat{\mathcal{R}}^{+}(R)\hat{T}_{kk'\dots}\hat{\mathcal{R}}(R) = \sum_l\sum_{l'}\dots R_{kl}R_{k'l'}\dots\hat{T}_{ll'\dots}$

Pozn.: invariantní podprostory na tenzorech II. řád.

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \quad T_{ik}$$

9 veličin ... skalár ... $T_{11}+T_{22}+T_{33} = \Delta$

vektor ... $(c_1, c_2, c_3) \leftarrow R$

i.R. tenzor 2. ř.

$$\begin{pmatrix} 0 & c_3 & -c_2 \\ -c_3 & 0 & c_1 \\ c_2 & -c_1 & 0 \end{pmatrix} \qquad A_{kl} = -A_{lk}$$

$$\underbrace{\frac{T_{kl}+T_{lk}}{2}}_{sym} + \underbrace{\frac{T_{kl}-T_{lk}}{2}}_{asym} \equiv T_{kl} = S_{kl} + A_{kl}$$

$$\bar{S} \equiv \frac{T_{kl}+T_{lk}}{2} - \frac{T_{kk}}{3}\delta_{kl} = \quad 0/3$$

$$\begin{pmatrix} S_{11} & S_{12} & S_{13} \\ & S_{22} & S_{23} \\ & & S_{33} \end{pmatrix}$$

5 nezávislých složek

$S_{33} = -S_{11} - S_{22}$

Reprezentace grupy rotací na prostoru matic 3×3

T_{kl} ... součin reprez. $\underline{R_{kk'}R_{ll'}} \equiv M_{kl,k'l'}$ $\quad$ 9×9

$\llcorner$ 9 dim prostor

$\longrightarrow$ rozloží na 3 inv. podpr.

- stopa ... $\frac{T_{kk}}{3}\delta_{kl}$. 1D
- A_{kl} 3D
- $\bar{S}_{kl}$ 5D

$\rightarrow D^{(0)}_{mm'} \quad D^{(1)}_{mm'} \quad D^{(2)}_{mm'}$

$$U^{+}MU = \begin{pmatrix} \boxed{D^{(0)}} & 0 & 0 \\ 0 & \boxed{D^{(1)}} & 0 \\ 0 & 0 & \boxed{D^{(2)}} \end{pmatrix} \begin{matrix} \leftarrow s \\ 9\times 9 \\ \leftarrow A \\ \leftarrow \bar{S} \end{matrix}$$

$\Big\}$ ireducibilní komponenty tenzoru II. řádu

Def.: Ireducibilním tenzorovým operátorem j-tého řádu (sférický tenzor) je $(2j+1)$-tice operátorů $T^{(j)}_{m}$ $m=-j,-j+1,\dots,j$, která se transformují jako

$$\boxed{\hat{R}^{+}(R)\,\hat{T}^{(j)}_{m}\,\hat{R}(R) = \sum_{m'=-j}^{j} D^{(j)*}_{mm'}(R)\,\hat{T}^{(j)}_{m'}}$$

Ekvivalentní definice:

IR. tenzoru

$$\boxed{\begin{aligned} [\hat{J}_z, \hat{T}^{(j)}_{m}] &= \hbar m \hat{T}^{(j)}_{m} \\ [\hat{J}_{\pm}, \hat{T}^{(j)}_{m}] &= \hbar\sqrt{(j\mp m)(j\pm m+1)}\,\hat{T}^{(j)}_{m\pm 1} \end{aligned}}$$

DK: $\boxed{[J_-, T_m] = \sum_{m'} T_{m'} \langle m' | J_- | m \rangle}$ $\pm$ $\quad 2i$

$J_+ = J_x + iJ_y$

$J_- = J_x - iJ_y$

rotace o úhel ε kolem osy $\vec{n}$

$$\hat{R}(R) = \exp\{-\tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J}\} = \hat{I} - \tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J} \leftarrow$$

$$D^{(j)*}_{mm'} \equiv \langle jm | [I - \tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J}] | jm' \rangle^{*} \rightarrow \langle jm' | I + \tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J} | jm \rangle$$

$$[\hat{I} + \tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J}]\,\hat{T}^{(j)}_{m}\,[I - \tfrac{i}{\hbar}\varepsilon\,\vec{n}\cdot\vec{J}] = \sum_{m'} (\;)\, T^{(j)}_{m'}$$

0. ř. $\quad T^{(j)}_{m} = T^{(j)}_{m}$

1. ř. $\quad [\vec{n}\cdot\vec{J}, T^{(j)}_{m}] = \sum_{m'} \langle jm' | \vec{n}\cdot\vec{J} | jm \rangle T^{(j)}_{m'}$

$\vec{n} = (1,0,0) \to J_x \qquad \vec{n} = (0,0,1) \dots J_z \qquad$ C.B.D.

$m \in -j, \dots, j$

Příklad: ⓪ .. $\boxed{\text{Skalár}} = \hat{T}^{(0)}_{00}$

$[\hat{J}_z, \hat{T}^{(0)}_{00}] = 0$

$[\hat{J}_\pm, T^{(0)}_{00}] = 0 \leftrightarrow [J_x, T^{(0)}_{00}] = [J_y, T^{(0)}_{00}] = 0$

skalár veličina je již operátor komutuje se $\forall \hat{J}_k$

$\hat{R}(R) \equiv \exp\{-\frac{i}{\hbar}\alpha \vec{n}\cdot\vec{J}\} \Rightarrow \quad R^+ T^0_{00} R = T^0_{00}$

$R^+ R = I$

1) vektor ... $\boxed{j=1}$

$\sqrt{(j \mp m)(j \pm m + 1)} = \sqrt{2}$ nebo 0

$[J_z, T^{(1)}_m] = \hbar m T^{(1)}_m$

$[J_\pm, T^{(1)}_m] = \begin{cases} 0 \\ \hbar\sqrt{2}\, T^{(1)}_{m\pm 1} \end{cases}$

kartéz. složky:

$[\hat{J}_k, \hat{V}_l] = i\hbar \varepsilon_{klm} \hat{V}_m$

$$\boxed{\begin{aligned} \hat{T}^{(1)}_0 &= \hat{V}_z \\ \hat{T}^{(1)}_{\pm 1} &= \mp \frac{\hat{V}_x \pm i\hat{V}_y}{\sqrt{2}} \end{aligned}}$$

ireducibilní složky vektoru

IR. slož. $\longleftrightarrow$ kartézské složky

$$\begin{pmatrix} -1/\sqrt{2} & -i/\sqrt{2} & 0 \\ +1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

2) $\boxed{j=2}$ ... $\hat{T}^{(2)}_{-2}, \hat{T}^{(2)}_{-1}, \hat{T}^{(2)}_0, \hat{T}^{(2)}_1, \hat{T}^{(2)}_2$ .. 5 složek

$m = -2, -1, \dots 2$

Tvrzení ... vekt. operátor $\hat{\vec{Q}} = (\hat{x}, \hat{y}, \hat{z})$ $\quad \hat{r} \equiv \sqrt{\hat{Q}_k \hat{Q}_k}$

sfér. harm. $\hat{r}^l Y_{lm}\left(\frac{\hat{\vec{Q}}}{r}\right)$ ... polynom. st. l v Q_1, Q_2, Q_3

$\hat{R}(R)\, \underbrace{Y_{lm}(\vec{Q})}_{|lm\rangle} = Y_{lm}(R^{-1}_{ij} Q_j) = \sum_{m'} D^{(l)*}_{m'm} Y_{lm'}(R)$

$\langle lm' | \hat{R} | lm\rangle \equiv D^{(l)}_{m'm}$

fix l ... invar. podpr.

operátor $\hat{Q}$ ... def. vekt. $\quad R^+ Q_k R = \sum R_{kk'} Q_{k'}$

$R \to R^{-1}$

$Y_{lm}(R_{kk'} Q_{k'}) = Y(R^{-1} Q R) = R(R^{-1}) Y_{lm}(Q) R(R^{-1})$

$\Rightarrow \quad R^+ Y_{lm}(\hat{Q}) R = \sum_{m'} D^{(l)*}_{m'm} Y^{(l)}_{m'}(\hat{Q})$

tj ∀ vektor. operátory $\hat{V}$ ... ∃ tenzorové operátory

$$\boxed{\hat{T}^{(\ell)}_m \equiv Y_{\ell m}(\hat{V})}$$

(0) ... $\hat{T}^{(0)}_{00} \equiv Y_{00}(\hat{V}) = \frac{1}{\sqrt{4\pi}}\hat{I}$

(1) ... $\hat{T}^{(1)}_m \equiv Y_{1m}(\hat{V})$

- $\sqrt{\frac{3}{4\pi}}\,\hat{V}_z$ $\quad m=0$
- $-\sqrt{\frac{3}{4\pi}}\,\frac{(\hat{V}_x+i\hat{V}_y)}{\sqrt{2}}$ $\quad m=1$
- $\sqrt{\frac{3}{4\pi}}\,\frac{(V_x-iV_y)}{\sqrt{2}}$ $\quad m=-1$

(2) $j=2$

$$r^2 Y_{20} = \sqrt{\frac{15}{8\pi}}\,\frac{2z^2-x^2-y^2}{\sqrt{6}}$$
$$r^2 Y_{2\pm1} = \sqrt{\frac{15}{8\pi}}\,(\mp1)\,z(x\pm iy)$$
$$r^2 Y_{2\pm2} = \sqrt{\frac{15}{8\pi}}\,\frac{1}{2}(x\pm iy)^2$$

$\Rightarrow$

$$\hat{T}^{(2)}_0 = \frac{1}{\sqrt{6}}\left(2\hat{V}_z^2-\hat{V}_x^2-\hat{V}_y^2\right)$$
$$\hat{T}^{(2)}_{\pm1} = \mp\, \underline{V_z(\hat{V}_x \pm i\hat{V}_y)}$$
$$\hat{T}^{(2)}_{\pm2} = \frac{1}{2}\left(\hat{V}_x \pm i\hat{V}_y\right)^2$$

OBECNĚ Tenzor operátor 2ř. $\underline{\hat{R}^+\hat{T}_{kl}\hat{R}} = \sum_{k'}\sum_{l'} R_{kk'}R_{ll'}\hat{T}_{k'l'}$

kartézské komp.

$$\hat{T}^{(0)}_0 = -\frac{1}{\sqrt{3}}\left(\hat{T}_{xx}+\hat{T}_{yy}+\hat{T}_{zz}\right) \quad \text{stopa}$$

$$\hat{T}^{(1)}_0 = \frac{i}{\sqrt{2}}\left(\hat{T}_{xy}-\hat{T}_{yx}\right)$$

$\hat{T}_{kl} \to \hat{A}_{kl} \to \hat{V}_k \to V^{(1)}_m$

$$\hat{T}^{(1)}_{\pm1} = \frac{i}{2}\left[\hat{T}_{zx}-\hat{T}_{xz} \pm i(\hat{T}_{zy}-\hat{T}_{yz})\right]$$

irr. složky antisym. části

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ir složky sym. bezest. č.

$$\hat{T}^{(2)}_0 = \frac{1}{\sqrt{6}}\left(2T_{zz}-T_{xx}-T_{yy}\right)$$
$$\hat{T}^{(2)}_{\pm1} = \frac{1}{2}\left[\mp(T_{zx}+T_{xz}) - i(T_{zy}+T_{yz})\right]$$
$$\hat{T}^{(2)}_{\pm2} = \frac{1}{2}\left[T_{xx}-T_{yy} \pm i(T_{xy}+T_{yx})\right]$$

Tenzorový součin

<u>Def</u>: nechť $\hat{S}^{(j_1)}_{m_1}$ a $\hat{T}^{(j_2)}_{m_2}$ jsou IR tenzorové operátory řádu j_1 a j_2:

$$\boxed{\hat{U}^{(j)}_m = \sum_{m_1 m_2} \langle j_1 j_2 m_1 m_2 | j m \rangle \hat{S}^{(j_1)}_{m_1} \hat{T}^{(j_2)}_{m_2}}$$

<u>Tvrzení</u>: $\hat{U}^{(j)}_m$ je IR tenzor řádu j

<u>DK</u>:
$$\underbrace{\mathcal{R}^+(R)\hat{U}^{(j)}_m \mathcal{R}(R)} = \sum_{m_1 m_2} \langle m_1 m_2 | j m \rangle \underbrace{\hat{\mathcal{R}}^+ \hat{S}^{(j_1)}_{m_1} \mathcal{R}}_{\sum_{m_1'} D^{(j_1)}_{m_1' m_1}(R^{-1}) S^{(j_1)}_{m_1'}} \underbrace{\mathcal{R}^+ \hat{T}^{(j)}_{m_2} \hat{\mathcal{R}}}$$

$$\left(D^{(j)}_{m_1 m_1'}(R)\right)^*$$

$$= \sum_{m_1 m_2} \sum_{m_1' m_2'} \langle m_1 m_2 | j m \rangle \underbrace{D^{(j_1)}_{m_1' m_1}(R^{-1}) D^{(j_2)}_{m_2' m_2}(R^{-1})}_{\sum_{(j'' m' m'')} \langle m_1' m_2' | j'' m' \rangle \langle m_1 m_2 | j'' m'' \rangle D^{(j'')}_{m' m''}} S^{(j_1)}_{m_1'} T^{(j_2)}_{m_2'}$$

$$\delta_{j j''} \delta_{m m''}$$

$$= \boxed{\sum_{m_1' m_2' m'}} \langle m_1' m_2' | j m' \rangle D^{(j)}_{m' m}(R^{-1}) \boxed{S^{(j_1)}_{m_1'} T^{(j_2)}_{m_2'}} \quad U^{(j)}_{m'}$$

$$= \underbrace{\sum_{m'} D^{(j)*}_{m m'} U^{(j)}_{m'}}$$ tj. $U^{(j)}_m$ splňuje def. IR tenzoru