QM I - 5 Bodová částice ve 3D a moment hybnosti

$$\mathcal{H} = L^2(\mathbb{R}^3) = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_1 \qquad \text{ÚSKO}$$

1) Operátor polohy

$$\boxed{\vec{X} = (\hat{X}_1, \hat{X}_2, \hat{X}_3)} \qquad \hat{X}_2 = \hat{I} \otimes X \otimes \hat{I}$$

→ souřad. reprez. ... $|x_1, x_2, x_3\rangle$

$$\langle x_1 x_2 x_3 | \psi \rangle = \psi(x_1, x_2, x_3) = \psi(\vec{x})$$

$$\langle \psi | \psi' \rangle = \int_{\mathbb{R}^3} \psi^*(x)\, \psi(x)\, d^3x \qquad \langle x_1 x_2 x_3 | x_1' x_2' x_3' \rangle =$$

2) Operátor hybnosti

$$\boxed{\vec{P} = (\hat{P}_1, \hat{P}_2, \hat{P}_3)} \quad \dots \ |p_1 p_2 p_3\rangle$$

$$\langle \vec{x} | \vec{p} \rangle = \langle x_1 | p_1 \rangle \langle x_2 | p_2 \rangle \langle x_3 | p_3 \rangle = \frac{1}{\sqrt{(2\pi\hbar)^3}}\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$$

$$\hat{\vec{P}}\, \psi(x) = \begin{pmatrix} \hat{P}_1 \psi(x) \\ \hat{P}_2 \psi(x) \\ \hat{P}_3 \psi(x) \end{pmatrix} = -i\hbar \nabla \psi(\vec{x})$$

$$-i\hbar \frac{\partial}{\partial x_i}$$

$$\langle \vec{p} | \vec{p}' \rangle = \delta(\vec{p} - \vec{p}') = \delta(p_1 - p_1')\,\delta(p_2 - p_2')\,\delta(p_3 - p_3')$$

$$\int d^3\vec{x}\, |\vec{x}\rangle\langle\vec{x}|$$

$$\int d^3\vec{x}\, \frac{1}{(2\pi\hbar)^3}\, e^{\frac{i}{\hbar}\vec{x}(\vec{p}' - \vec{p})} = \frac{1}{2\pi} \int \frac{dx_1}{\hbar}\, e^{2\pi i \left(\frac{x_1}{h}\right)(p_1' - p_1)} \cdot \, _2 \, _3$$

$$\int_{-\infty}^{\infty} e^{2\pi i k x}\, dx = \delta(k)$$

→ $|p_1 p_2 p_3\rangle$ -- $\psi(p_1, p_2, p_3)$

$$\hat{\vec{P}} = \vec{P}\, \psi(\vec{p}) \qquad \hat{X}\psi = i\hbar \nabla \psi(\vec{p})$$

3) Energie volné č. + směr hybnosti

$$\hat{H}_0 = \frac{\vec{P}^2}{2m} = \frac{\hat{P}_1^2 + \hat{P}_2^2 + \hat{P}_3^2}{2m}$$

$$\hat{H}_0 = \frac{1}{2m} \sum_\alpha \hat{P}_\alpha \hat{P}_\alpha \qquad \hat{\vec{n}} = \frac{\hat{\vec{P}}}{\hat{P}} \qquad \frac{\hat{p}_1}{\sqrt{\hat{p}_1^2 + \hat{p}_2^2 + \hat{p}_3^2}}$$

$$n_1^2 + n_2^2 + n_3^2 = 1 \qquad \boxed{\hat{H}_0, \hat{\vec{n}}} \ \text{ÚSKO}$$

$$[\hat{H}_0, \hat{P}_\alpha] = 0 \qquad \sim |E, \vec{n}\rangle$$

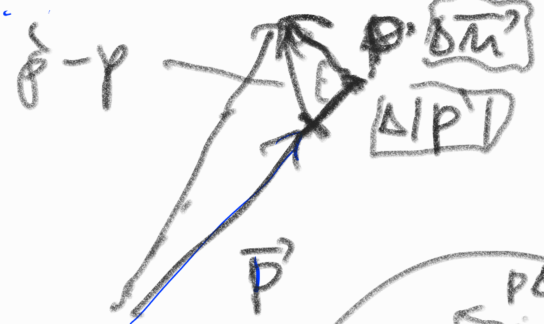
$$\hat{H}_0 |E, \vec{n}\rangle = E |E, \vec{n}\rangle$$

$$\hat{\vec{n}} |E, \vec{n}\rangle = \vec{n} |E, \vec{n}\rangle$$

$\vec n,\ E \to p_E = \sqrt{2mE}$ $\boxed{\vec p_{E,\vec n} = p_E \vec n}$

$|E,\vec n\rangle = \eta\,|\vec p\rangle$ $\boxed{\langle E,\vec n | E',\vec n'\rangle = \delta(E-E')\,\delta^{(2)}(\vec n-\vec n')}$

$$\langle E,\vec n|E'\vec n'\rangle = |\eta|^2 \langle \vec p\,|\,\vec p'\rangle = |\eta|^2\,\delta^{(3)}(\vec p-\vec p')$$

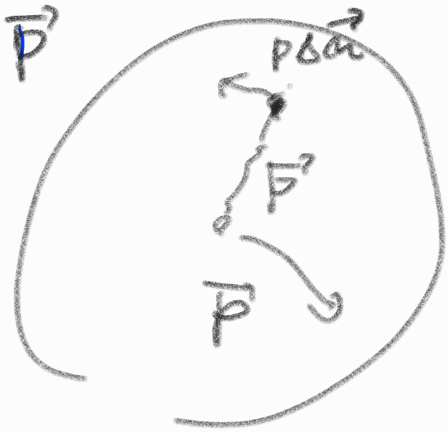


$$|\eta|^2\,\delta(p-p')\,\delta^{(2)}_{\theta}(p(\vec n-\vec n'))$$

$$\delta(f(x)) = \sum_i \frac{\delta(x-x_i)}{|f'(x_i)|}$$

$p \approx \sqrt{2mE}$ $\quad \frac{m}{p} = p'_E = \frac{1}{2}\,2m\,\frac{1}{\sqrt{2mE}}$

$$\frac{p}{m}\,\delta(E-E')$$



$$\delta^{(2)}(p(\vec n-\vec n')) = \frac{\delta^{(2)}(\vec n-\vec n')}{p^2}$$

$$\langle E\vec n|E'\vec n'\rangle = |\eta|^2\,\frac{1}{mp}\,\delta(E-E')\,\delta^{(2)}(\vec n-\vec n')$$

$\dots\ \eta = \sqrt{mp}$

závěr: $\underbrace{\{H_0, \vec n\}}_{\text{ÚSKO}}$ -- $\boxed{|E\vec n\rangle = \sqrt{mp}\,|\vec p\rangle = \sqrt{\frac{mp_E}{(2\pi\hbar)^3}}\, e^{\frac{i}{\hbar}\vec x\,\underbrace{\vec n\sqrt{2mE}}_{\vec p_E}}}$ BÁZE

pozn.: bod. částici v 3D … $\underbrace{\mathcal H_x \otimes \mathcal H_y \otimes \mathcal H_z}$ ($\hat x$, $\hat y$, $\hat z$)

E, n $\quad \mathcal H = \underbrace{\mathcal H_r}_{1D} \otimes \underbrace{\mathcal H_S}_{2D}$ ($\hat{\vec n}$) $\quad S_2 = \{\vec x \in \mathbb R^3, \|x\| = 1\}$

kvantování radiálních a úhlových stupňů volnosti

$L^2(0,\infty)$ $\quad H_0 \quad$ $L^2(S_2)$

$\psi(r)$ $\quad\quad \psi(\vec n)$

4) Orbitální moment hybnosti

(alternativní kvantování na $L^2(S_2)$ -- úhlové stupně volnosti)

klas $\vec{L} = \vec{x} \times \vec{p}$ $\quad \hat{L}_\alpha = \varepsilon_{\alpha\beta\gamma} \hat{x}_\beta \hat{p}_\gamma \quad \vec{L} = (\hat{L}_1, \hat{L}_2, \hat{L}_3)$

$$\left.\begin{aligned} [\hat{\vec{x}}, \hat{\vec{p}}] &= i\hbar \hat{I} \\ [\hat{x}_\alpha, \hat{p}_\beta] &= i\hbar \hat{I} \delta_{\alpha\beta} \end{aligned}\right\} \to [\hat{L}_\alpha, \hat{L}_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} \hat{L}_\gamma \leftarrow S_i$$

$$[\hat{L}_1, \hat{L}_2] = i\hbar \hat{L}_3$$

$$[\hat{L}^2, \hat{L}_1] = \underbrace{[L_1^2, L_1]}_{0} + [L_2^2, L_1] + [L_3^2, L_1] = 0$$

$\hat{L}^2 = L_1^2 + L_2^2 + L_3^2$

$[L_2^2, L_1] = L_2 [L_2, L_1] + [L_2, L_1] L_2$

$$\boxed{[L^2, L_\alpha] = 0} \quad \alpha = 1, 2, 3$$

$$\mathcal{H} = L^2(\mathbb{R}^3) = \mathcal{H}_r \otimes \mathcal{H}_{S_2} \to \text{ÚSKO } \{\hat{A}, \hat{L}^2, \hat{L}_z\}$$

$\mathcal{H}_r$: $\hat{A}$; $\mathcal{H}_{S_2}$: $L^2, \hat{L}_z$

př... $\hat{H}_0$

Delší odbočka: Kvantová teorie momentu hybnosti

pozorov. $\hat{J}_\alpha^+ = \hat{J}_\alpha$

OBECNĚ: Def: $\{\hat{J}_1, \hat{J}_2, \hat{J}_3\}$ se nazývá mom. hybn.

pakud $[\hat{J}_\alpha, \hat{J}_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} \hat{J}_\gamma$

- def. operátor kvadrátu délky $\hat{\vec{J}}$ .. $\hat{J}^2 \equiv J_\alpha J_\alpha$

$$[J^2, J_\alpha] = 0$$

- $\exists$ spol. sada vl. v. $\quad (|\alpha \beta m\rangle)$

$$\hat{J}^2 |\beta, m\rangle = \hbar^2 \beta |\beta, m\rangle$$
$$\hat{J}_3 |\beta, m\rangle = \hbar m |\beta, m\rangle$$

? σ_{J^2, J_z} .. $\{(\beta, m)\}$?

- $$\beta = \langle \beta, m | \frac{J^2}{\hbar^2} | \beta m\rangle = \langle \beta m | \underbrace{\left(\frac{J_1}{\hbar}\right)^2}_{\geq 0} + \underbrace{\left(\frac{J_2}{\hbar}\right)^2}_{\geq 0} + \underbrace{\left(\frac{J_3}{\hbar}\right)^2}_{\geq 0} |\beta m\rangle \geq 0$$

$$\left\| \frac{\hat{J}_3 |\beta, m\rangle}{\hbar} \right\|^2 \geq 0$$

$$\beta = \emptyset + \emptyset + \frac{\langle \beta m | J_3^2 | \beta m \rangle}{\hbar^2} = \emptyset + \emptyset + m^2 \geq 0$$

$\boxed{\beta \geq m^2 \geq 0}$ ... spektrum J_3 je omezené

omez. zdola

$$\boxed{-\sqrt{\beta} \leq m \leq \sqrt{\beta}}$$

• posunovací operátory

$J_1 \quad J_2 \quad i\hbar J_3$

$J_+ = J_1 + iJ_2 \qquad J_+^\dagger = J_-$

$J_- = J_1 - iJ_2 \qquad J_-^\dagger = J_+$

$$[J_3, J_+] = \underbrace{[J_3, J_1]}_{i\hbar J_2} + i\underbrace{[J_3, J_2]}_{-i\hbar J_1} = \hbar(J_1 + iJ_2) = \boxed{\hbar J_+}$$

$$\boxed{[J_3, J_-] = -\hbar J_-} \qquad \boxed{[J_+, J_-] = 2\hbar J_3}$$

$J_+ |\beta m\rangle = |\psi\rangle$? $\quad \underline{[J_+, J^2] = 0}$ ... $\Rightarrow$ $|\psi\rangle$ je vl. v. J^2 ... β

$$\underline{J_3 |\psi\rangle} = \underbrace{J_3 (J_+}_{J_+ J_3 + \underbrace{[J_3, J_+]}_{\hbar J_+}} |\beta m\rangle) = \hat{J}_+ \underbrace{\hat{J}_3 |\beta m\rangle}_{\hbar m |\beta m\rangle} + \hbar J_+ |\beta m\rangle = \hbar (m+1) \underbrace{J_+ |\beta\rangle}_{\psi}$$

$J_3 |\psi\rangle = \hbar (m+1) |\psi\rangle$ tj $\boxed{|\psi\rangle \sim |\beta (m+1)\rangle}$

$J_- |\beta m\rangle \qquad [J_-, J^2] = 0 \quad \Rightarrow \quad J_- |\beta m\rangle$ ... β

$$J_3 J_- = J_- J_+ + \underbrace{[J_3, J_-]}_{= -\hbar J_-} \quad \Rightarrow \quad J_- |\beta m\rangle \sim |\beta (m-1)\rangle$$

• omezenost J_3 $\Rightarrow$ max. $m = j$

$\| J_+ |\beta j\rangle \|^2 = 0; \qquad \langle \beta j | \beta j \rangle = 1$

$$\underline{\langle \beta j | J_- J_+ | \beta j \rangle} = \langle \beta j | \hbar^2 \beta - \hbar^2 j^2 - \hbar^2 j | \beta j \rangle = \underbrace{\hbar^2 (\beta - j^2 - j) = 0}_{\beta = j^2 + j}$$

$$\boxed{J_- J_+ = J^2 - J_3^2 - \hbar J_3}$$

$$\boxed{J_+ J_- = J^2 - J_3^2 + \hbar J_3}$$

$$(\hat{J}_1 - i\hat{J}_2)(\hat{J}_1 + i\hat{J}_2) = \underbrace{J_1^2 + J_2^2}_{J^2 - J_3^2} + i\underbrace{(\hat{J}_1\hat{J}_2 - \hat{J}_2\hat{J}_1)}_{i\hbar J_3} \quad ✓$$

$\beta = j(j+1)$ .. max hodn. $m = j$

- minimální hodnota $m = k$

$$\| \hat{J}_- |\beta k\rangle \|^2 = 0$$

$$\langle \beta k | J_+ J_- | \beta k\rangle = \langle \beta k | J^2 - J_3^2 + \hbar J_3 | \beta k\rangle = \hbar^2 (\underset{j(j+1)}{\beta} - k^2 + k) = 0$$

$$j(j+1) = k^2 - k \Rightarrow k = \begin{cases} \cancel{j+1} \\ -j \end{cases}$$

$\boxed{\text{závěr}}$: β – j – $-j$

- $m = -j, -j+1, -j+2, \dots, j \Rightarrow j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\}$

$2j \in \mathbb{N}_0 \quad \forall \beta = \underline{j(j+1)}$

přeznačení .. $|\beta m\rangle \rightarrow \underline{|j m\rangle}$ ..

$$\boxed{\begin{aligned} \hat{J}_3 |jm\rangle &= \hbar m |jm\rangle \\ \hat{J}^2 |jm\rangle &= \hbar^2 j(j+1) |jm\rangle \end{aligned}}$$

$j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots\}$

$m = -j, -j+1, \dots, j$

PŘ: • částice se spinem $\frac{1}{2}$ ... $\vec{J} = \vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right)$

$$[\sigma_\alpha, \sigma_\beta] = 2i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma$$

$|+\rangle \equiv |jm\rangle = |\tfrac{1}{2}\, +\tfrac{1}{2}\rangle$

$|-\rangle \equiv |\tfrac{1}{2}\, -\tfrac{1}{2}\rangle$

$m = -\frac{1}{2}, \frac{1}{2}$

$$\sigma_{J^2} = \{\hbar^2 j(j+1);\ j = \tfrac{1}{2}\}$$

* orbitální moment hybnosti ...

* normalizace působení $\hat{J}_\pm$

$$J_+ |jm\rangle = \eta |j(m+1)\rangle$$

$$\| J_+ |jm\rangle \|^2 = \langle jm| J_- J_+ |jm\rangle = \langle jm| J^2 - J_3^2 - \hbar J_3 |jm\rangle$$

$$= \hbar^2 j(j+1) - \hbar^2 m^2 - \hbar^2 m = \hbar^2 \left[j(j+1) - m(m+1) \right]$$

$$\boxed{J_+ |jm\rangle = \hbar \sqrt{j(j+1) - m(m+1)}\, |j(m+1)\rangle = \hbar \sqrt{(j-m)(j+m+1)}\, |j(m+1)\rangle}$$

$e^{i\pi}$

$J_+ |jj\rangle = 0$

$|jm\rangle$

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

příště

* ... $\vec{J} = \vec{S}$ ... $j = \frac{1}{2}$ ... $j > \frac{1}{2}$
* $\vec{J} = \vec{L}$