QMI - 5 částice ve 3D - orbitální moment hybnosti, kulové fce

OPAKOVÁNÍ:

$[\hat{L}_\alpha, \hat{L}_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} \hat{L}_\gamma \Rightarrow [\hat{L}^2, \hat{L}_z] = 0 \Rightarrow$ $L^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle$, $L_z |lm\rangle = \hbar m |lm\rangle$

$l = 0, 1, 2, 3, \dots \quad m = -l, -l+1, \dots, l \quad (2l+1)\times$

$\partial_\varphi = \frac{\partial}{\partial \varphi}$

$$\hat{L}_x = -i\hbar(y\partial_z - z\partial_y) = -i\hbar(-\sin\varphi\,\partial_\theta - \cos\varphi\cot\theta\,\partial_\varphi)$$
$$\hat{L}_y = -i\hbar(z\partial_x - x\partial_z) = -i\hbar(\cos\varphi\,\partial_\varphi - \sin\varphi\cot\theta\,\partial_\varphi)$$
$$\hat{L}_z = -i\hbar(x\partial_y - y\partial_x) = -i\hbar\,\partial_\varphi$$

$$L_\pm = \hbar e^{\pm i\varphi}[\pm\partial_\theta + i\cot\theta\,\partial_\varphi]$$

$$L^2 = -\hbar^2(r^2\Delta - \partial_{rr} - 2r\partial_r)$$

$\Rightarrow$ charakterizace $\langle\vec{x}|lm\rangle$ ($= Y_{lm}(\vec{x})$) jako polynomů na 1-sféře:

- homog. polynom st. l $\quad p_l(x,y,z) = \mathcal{L}(x^a y^b z^c)$, $a+b+c = l$
- $\Delta p_l(x,y,z) = 0 \quad \Rightarrow \quad L^2 p_l = \hbar^2 l(l+1) p_l$
- prostor takových p_l invariantní působení $\hat{L}_\alpha$

$\rightarrow$ tento prostor má dimenzi $(2l+1)$ stejně jako $|lm\rangle\ \forall m$

$\forall$ homogen. poly p_l: $\Delta p_l = 0 \equiv$ vl. podpr. L^2 - $\hbar^2 l(l+1)$

$\mathcal{L}(\forall \langle\vec{x}|lm\rangle$ pro fix l a $\forall m) = \mathcal{L}(\forall p_l$ st l; $\Delta p = 0)$

Vlastní stavy $\langle\vec{x}|lm\rangle \equiv Y_{lm}(\vec{x})$, kulové funkce

separace prom. - $Y_{lm}(\theta,\varphi) = f(\theta)\,g(\varphi)$ $\quad f$ poly st $l-|m|$

$\hat{L}_z g(\varphi) = -i\hbar\,\partial_\varphi g(\varphi) = \hbar m\, g(\varphi) \rightarrow \boxed{g(\varphi) = e^{im\varphi}}$

$e^{im\varphi} = (\cos\varphi + i\sin\varphi)^m = \varphi$ část výrazu $(x \pm iy)^{|m|}$

$x = r\cos\varphi\sin\theta \qquad y = r\sin\varphi\sin\theta \qquad$ polynom st m

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

~~$L_\pm |lm\rangle$~~ $\quad \left[-\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} - \frac{m^2}{\sin^2\theta} \right] f(\theta) = l(l+1) f(\theta) \right]$

$f(\theta)$ -- polynom st $l - |m|$ $\quad x\, y\, z$

$m=1$ $\quad$ subst $z = \cos\theta$

$$\Rightarrow \quad \left\{ \frac{d}{dz} (1-z^2) \frac{d}{dz} + \lambda - \frac{m^2}{1-z^2} \right\} f(\theta) = 0 \qquad \lambda = l(l+1)$$

$$P_l^m(\xi) \sim \frac{1}{2^l l!} (1-\xi^2)^{m/2} \frac{d^{l+m}}{d\xi^{l+m}} (\xi^2 - 1)^l \qquad P_l^m(\cos\theta)$$

shrnutí: $\langle \vec{x} | lm\rangle = Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\varphi}$

Kulové funkce, sférické harmoniky (spherical harmonics)

ON: $\langle lm | l'm'\rangle = \int_{S_2} Y^*_{lm}(\vec{n})\, Y_{l'm'}(\vec{n})\, d\Omega = \delta_{ll'} \delta_{mm'}$

$\mathcal{H} = L(\mathbb{R}^3) = \mathcal{H}_r \otimes \mathcal{H}_{S_2}$ $\qquad \vec{n} = \frac{\vec{x}}{r} = (\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$ $\quad r=1$

$d\Omega = \sin\theta\, d\theta\, d\varphi = (d\cos\theta)\, d\varphi$ $\qquad h_\theta = r$, h_φ

úplnost na

$\sum_{lm} |lm\rangle\langle lm| = \hat{1}_{\mathcal{H}_{S_2}}$ $\qquad |x'\rangle$ $\qquad \langle x | x'\rangle \; \ldots \; \delta_2(x - x')$ $\quad |\vec{n}\rangle$ $\quad |x| = 1$, $\vec{x} \in S_2$, $\vec{n}$

$d\varphi$

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\vec{n})\, Y^*_{lm}(\vec{n}') = \delta_2(\vec{n} - \vec{n}') = \frac{\delta(\theta-\theta')\,\delta(\varphi-\varphi')}{|\sin\theta|}$$

$ds = h_\varphi d\varphi$

$\delta(kx) = \frac{\delta(x)}{|k|}$ $\qquad \int \delta_2(\vec{n} - \vec{n}')\, \phi(\vec{n}')\, d\Omega = \phi(\vec{n})$

Odvození tvaru $Y_{lm}(\theta, \varphi)$ z algebr. vlast. $\hat{L}_\pm |lm\rangle$

$m =$

$L_+ |l\,l\rangle = 0$ $\qquad 0 = L_- Y_{l-l}(\theta\varphi) = \hbar e^{-i\varphi} \left[-\partial_\theta + i \frac{\cos\theta}{\sin\theta} \partial_\varphi \right] f(\theta) e^{-il\varphi}$

$L_- |l\,{-l}\rangle = 0$

$e^{im\varphi}$, $m = -l$ $\qquad \left[-\frac{d}{d\theta} + l \frac{\cos\theta}{\sin\theta} \right] f(\theta) = 0$

$\frac{f'}{f} = l\frac{\cos\theta}{\sin\theta}$ ... $f(\theta) = c_l(\sin\theta)^l$

$Y_{l-l} = c_l(\sin\theta)^l e^{-il\varphi} = c_l \sin\theta^l(\cos\varphi - i\sin\varphi)^l$

$\overline{Y_{ll}} = c_l(\sin\theta\cos\varphi - i\sin\varphi\sin\theta)^l = c_l(x-iy)^l$ $e^{-il\varphi}$

$1 = \int |Y_{l-l}|^2 d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, |c_l|^2 \sin\theta^{2l} = 1$

2π

$I_l = \int_0^{\pi} \sin\theta\, d\theta\, (\sin\theta^2)^l$ ($d\cos\theta$, z; $1-\cos^2\theta$, $1-z^2$)

$I_l = \frac{2^{2l+1}(l!)^2}{(2l+1)!}$ $e^{i\delta}$

$c_l = \frac{1}{\sqrt{2\pi I_l}} = \frac{-1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}$

$Y_{l-l}(\theta,\varphi) = c_l(x-iy)^l$ ... $Y_{l0}(\theta,\varphi) > 0$ $\theta = 0$

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

$L_+ = \hbar e^{i\varphi}\left[\frac{\partial}{\partial\theta} - m\frac{\cos\theta}{\sin\theta}\right]$. $e^{im\varphi} f_l(\theta)$

Quantum Mechanics → Cohen-Tannodji $z = \cos\theta$

$$Y_{lm}(\theta,\varphi) = \frac{(-1)^{l+m}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, e^{im\varphi}(\sin\theta)^m \frac{d^{l+m}}{(d\cos\theta)^{l+m}}(\sin\theta)^{2l}$$

Přidružené Legendreova fce → $P_l^m(z)$

pozn.: $Y_{l0}(\theta)$ ... Legendreův polynom ($\cos\theta$) z

$$Y_{l0}(\theta) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}\frac{d^l}{dz^l}(1-z^2)^l\Big|_{z=\cos\theta} = \sqrt{\frac{2l+1}{4\pi}}P_l(z)$$

$\psi(r,\theta,\varphi)$ $\partial_\varphi \psi = 0$ $e^{im\varphi}$ $m = 0$

↳ $h(r) f(\theta)$

$$\delta_{\ell\ell'} = \int Y_{\ell 0}(\vec{n})\, Y^*_{\ell' 0}(\vec{n})\, d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta\, \frac{2\ell+1}{4\pi} P_\ell(z) P_{\ell'}(z)$$

$z = \cos\theta$

$$\Rightarrow \text{OG} \int_{-1}^{1} P_\ell(z) P_{\ell'}(z)\, dz = \frac{2}{2\ell+1}\delta_{\ell\ell'} \ldots \quad \text{LHO} \quad H_n(x)$$

$$\text{OG} \quad \int_{-\infty}^{\infty} H_n(x) H_{n'}(x)\, e^{-x^2} dx = A_n \delta_{nn'} \quad \text{Hermite}$$

pozn.) symetrie ... parita

$$Y_{\ell m}(-\vec{n}) = Y_{\ell m}(\vec{n})(-1)^\ell$$

$x \to -x \quad y \to -y, \quad z \to z$

$\vec{x} \to -\vec{x}$

$$P_\ell(\lambda x, \lambda y, \lambda z) = \lambda^\ell P_\ell(x,y,z)$$

$\lambda = -1$

$$Y^*_{\ell m}(\vec{n}) = (-1)^m Y_{\ell -m}(\vec{n})$$

$f(\theta)\, g(\varphi)^*$

$m \quad -m$

$|\hat{L}_z|$ -- $Y_{\ell m}$ -- $\hbar|m|$ $\quad e^{im\varphi}$ $\quad (+) \to (-)$

$- Y_{\ell -m} \quad Y^*_{\ell m} \quad \theta \quad \varphi$

$$C_{\ell m} = \frac{1}{\sqrt{2}}(Y_{\ell m} + Y^*_{\ell m}) \equiv \sqrt{2}\, \mathrm{Re}\, Y_{\ell m} \quad \text{Def.} \quad \text{liší} \quad (-1)^{m+1}$$

$$S_{\ell m} = \frac{1}{i\sqrt{2}}(Y_{\ell m} - Y^*_{\ell m}) \equiv \sqrt{2}\, \mathrm{Im}\, Y_{\ell m}$$

$s \quad 1p \ldots \quad p_x \quad p_y \quad p_z \quad d$

$Y_{00} \quad e^{\pm i\varphi} \quad Y_{10} \ldots \quad \cos\theta \sim z$

$$Y_{\ell m} = (x \pm iy)$$

$x \leftarrow C_{\ell m}$, $y \leftarrow S_{\ell m}$

ÚSKO 3D

$\hat{\vec{X}}$; $\hat{\vec{P}}$; $H_0 = \frac{p^2}{2m}$, $\vec{n}$ $\quad$ ~~$\vec{n}\ \vec{p}$~~ $\quad L^2, L_z$

4) ÚSKO $\hat{L}^2, \hat{L}_z, \hat{A}$

$$[\hat{A}, \hat{L}_\alpha] = 0 \Rightarrow [\hat{A}, \hat{L}^2] = 0$$

$\Rightarrow [\hat{A}, \hat{L}_\pm] = 0$ $\quad \hat{L}_x \pm i\hat{L}_y = \hat{L}_\pm$ $\quad |a, l m\rangle$

$\hat{A}|a_i\rangle = a|a_i\rangle$ ... $\hat{L}_\pm |a\rangle$, ... také vl. v. $\hat{A}$ ... a

$L^2 |alm\rangle = \hbar l(l+1)|alm\rangle$

$L_z |alm\rangle = \hbar m |alm\rangle$

$\hat{A} |alm\rangle = a^{(l)} |alm\rangle$ $\quad$ ale $a^{(l)}$ nezávisí na m

4a) $A = \hat{H}_0 \equiv \hat{p}^2/2m$, L^2, L_z $\quad H_0|Elm\rangle = E|Elm\rangle$

$\hat{p}$ - reprezentace ... vl. v. $\hat{p}^2 = p_x^2 + p_y^2 + p_z^2$

$[H_0, L_z] = 0$ $\quad [p_\alpha, p_\beta] = [x_\alpha, x_\beta] = 0$ $\quad [z, p_z] = i\hbar$

$[x_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$

$\frac{1}{2m}[p_x^2 + p_y^2 + p_z^2, x p_y - y p_x] =$

$= \frac{1}{2m}\left([p_x^2, x p_y] - [p_y^2, y p_x]\right) = \frac{1}{2m}\left(x[p_x^2, p_y] + [p_x^2, x]p_y - y[p_y^2, p_y] - [p_y^2, y]p_x\right)$

$[A, BC] = [A, B]C + B[A, C]$

$= \frac{1}{2m}\left([p_x^2, x]p_y - [p_y^2, y]p_x\right) = \frac{1}{2m}\left(-2i\hbar p_x p_y - (-2i\hbar p_y)p_x\right)$

$[p_y^2, y] = -2i\hbar p_y$

$p_x[p_x, x] + [p_x, x]p_x = -2i\hbar p_x$ $\quad$ (kde $[p_x, x] = -i\hbar$) $\quad = 0$

L^2, L_z v p reprezentaci ?? $\quad |lm\rangle$

$L_\pm$, $\quad L_z = -i\hbar(x\partial_y - y\partial_x)$ $\quad \langle\vec{p}|lm\rangle$

$x \to i\hbar\partial_{p_x}$, $\quad \partial_y \to p_y$ $\quad L_z \equiv -i\hbar(p_x\partial_{p_y} - p_y\partial_{p_x})$

$\Rightarrow$ stejné difrc. $\begin{matrix} L^2|lm\rangle \\ L_z|lm\rangle \end{matrix}$ $\rightarrow$ stejné řeš. $Y_{lm}(\vec{p})$

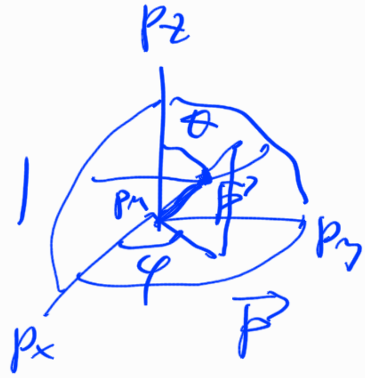
$|Elm\rangle$ -- $\underline{f(p_r)}\, Y_{lm}(\theta, \varphi)$ $\qquad$ $p_x = p_r \cos\varphi \sin\theta$

atd.

$$p_r \equiv \sqrt{p_x^2 + p_y^2 + p_z^2}$$

? $f(p_r)$ -- vl. fce $H_0 = \frac{p^2}{2m} = \frac{p_r^2}{2m} = E$

$$f(p_r) \sim \delta\left(p_r - \sqrt{2mE}\right)$$



$$\langle \vec{p} | Elm \rangle = N\, \delta\left(\frac{p^2}{2m} - E\right) Y_{lm}\left(\frac{\vec{p}}{p_r}\right)$$

$$\langle Elm | E'l'm' \rangle =$$