QM I - 5 - Bodová částice 3D – ÚSKO L^2, L_z, H_0

ÚSKO $L_2(\mathbb{R}^3)$: $\vec{x}, \vec{p}, \{L^2, L_z, H_0\}$ ...

$$\frac{p^2}{2m} = E \qquad p_E = \sqrt{2mE}$$

4) $\{\hat{H}_0, \hat{L}^2, \hat{L}_z\}$ $|E, l, m\rangle$

$$\hat{H}_0 |Elm\rangle = E|Elm\rangle$$
$$\hat{L}^2 |Elm\rangle = \hbar^2 l(l+1)|Elm\rangle$$
$$\hat{L}_z |Elm\rangle = \hbar m |Elm\rangle$$

4a) p-reprez. stejně jak x-repr.

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

$$\vec{p} = (p\cos\varphi\sin\theta,\ p\sin\varphi\sin\theta,\ p\cos\theta) = (p_x, p_y, p_z)$$

- $\langle Elm|E'l'm'\rangle = \delta(E-E')\,\delta_{ll'}\,\delta_{mm'}$

$$\int d^3p\, |N|^2 \delta\!\left(E - \frac{p^2}{2m}\right) Y^*_{lm}\!\left(\frac{\vec{p}}{p}\right) \delta\!\left(E' - \frac{p^2}{2m}\right) Y_{l'm'}\!\left(\frac{\vec{p}}{p}\right)$$

$$p^2 d\Omega\, dp \quad \Big| \quad = |N|^2 \int_0^\infty p^2 dp\, \underbrace{\delta\!\left(E - \frac{p^2}{2m}\right)\delta\!\left(E' - \frac{p^2}{2m}\right)}_{\delta(E-E')} \underbrace{\int d\Omega\, Y^*_{lm}(\hat{p})\, Y_{l'm'}}_{\delta_{ll'}\delta_{mm'}}$$

$$E = \frac{p_E^2}{2m}$$

$$\delta\!\left(\frac{p_E^2}{2m} - \frac{p^2}{2m}\right) = 2m\,\delta\big((p_E - p)(p_E + p)\big) = \frac{2m}{2p_E}\,\delta(p_E - p) \qquad p \to p_E$$

$$\delta(kx) = \frac{\delta(x)}{|k|}$$

$$\langle Elm|E'l'm'\rangle = |N|^2 \frac{m}{p_E} p_E^2\, \underbrace{\delta\!\left(E' - \frac{p_E^2}{2m}\right)}_{E} \delta_{ll'}\delta_{mm'}$$

$$N = \frac{1}{\sqrt{p_E m}}$$

závěr: $$\langle \vec{p}|Elm\rangle = \frac{1}{\sqrt{p_E m}}\,\delta\!\left(E - \frac{p^2}{2m}\right) Y_{lm}(\hat{p})$$

4b) ÚSKO $\{H_0, L^2, L_z\}$ ~ $|Elm\rangle$ v x-reprez.

motivace → volná částice .. startovací bod

- konstrukce modelů z po částech konst. potenciálů

$\psi_{Elm}(\vec{p})$ $\quad p \to x \quad$ $\psi_{Elm}(\vec{x}) = \int d^3p \, \langle \vec{x}|\vec{p}\rangle \langle p|Elm\rangle$

$\langle x| \; \uparrow \; |\psi\rangle \qquad \langle \vec x|\vec p\rangle \to \frac{1}{\sqrt{(2\pi\hbar)^3}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$

$\mathbb{1} = \int d^3p \, |p\rangle\langle p|$

$\vec{r} \equiv \vec{x} \equiv (x, y, z) = (r, \theta, \varphi)$

x_1, x_2, x_3

$$\boxed{e^{i\vec{k}\cdot\vec{x}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) \, Y^*_{lm}(\vec{k}) \, Y_{lm}(\vec{x})}$$

sférické cylindrické fce

sférické Besselovy fce

$|lm\rangle \quad \vec{L} \quad L_+ \, L_-$

$Y_{lm}(\vec{k}) \xrightarrow{p} i^l Y_{lm}(\vec{p})$

přímé nalezení $|Elm\rangle$ v x-reprezentaci $\qquad \psi_{Elm}(\vec{x}) = \langle \vec{x}|Elm\rangle$

$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \quad \ldots k_E = \frac{p_E}{\hbar} \quad \ldots k \qquad \frac{\vec{x}}{r} \qquad \psi_{klm}$

$\hat{L}^2, L_z \quad \ldots \quad \boxed{\psi_{klm}(\vec{x}) = R_{kl}(r) Y_{lm}(\theta, \varphi)} \qquad L_\pm \ldots \theta, \varphi$

- poznámka: zavedení radiální vln. funkce

$\psi_1(\vec{x}), \quad \psi_2(\vec{x}) \quad \ldots \quad \langle \psi_1|\psi_2\rangle = \int r^2 dr \, R_1^*(r) R_2(r) \int d\Omega \, Y_1^* Y_2$

$R_1(r) Y_1(\theta,\varphi) \qquad R_2(r) Y_2(\theta,\varphi)$

$\frac{1}{r}\chi_1 \qquad \frac{1}{r}\chi_2$

$\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_{S_2}$

$\int_0^\infty dr \, \chi_1^*(r) \chi_2(r)$

$\chi \equiv r R(r)$

skal. souč. na $L^2_0((0,\infty))$

(později uvidíme navíc $\chi(r \to 0) = 0$)

BÚNO

$\psi_{klm}(\vec{x}) = \frac{1}{r}\chi_{kl}(r) Y_{lm}(\theta,\varphi) \qquad L^2, L_z$

$H_0 \psi_{klm}(\vec{x}) = -\frac{\hbar^2}{2m} \Delta \psi_{klm} = -\frac{\hbar^2}{2m} \frac{1}{r^2}\left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - l(l+1)\right]\psi \quad +V$

$= \frac{\hat{p}^2}{2m} \qquad p = -i\hbar\nabla$

$-\frac{L^2}{\hbar^2 r^2} \to \hbar^2 l(l+1) \qquad \frac{1}{r}\chi Y \qquad =$

$H_0\psi = E\psi = \frac{\hbar^2 k^2}{2m} \frac{1}{r}\chi Y$

$$-\frac{1}{r^2}\left[\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - l(l+1)\right]\boxed{\frac{1}{r}\chi(r)} = k^2 \frac{1}{r}\chi(r) \quad \Big| \cdot (-1)\;\; r^2 dr$$

R

$$\boxed{\frac{d^2}{dr^2}}$$

centrifugální člen

$$\rightarrow \boxed{\chi''(r) + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi(r) = 0} \quad \text{radiální (rSR)}$$

pro volnou č.

pozn. interagující částice — $H_0 \rightarrow H_0 + V(r)$

$$\frac{d}{dr^2} \qquad \frac{2mV}{\hbar^2} \qquad r \rightarrow kr = z$$

- řešení pro $l=0$: 1D SR ... $r=0$ $\quad \psi(x<0)=0$

$$\chi(r) = A \sin kr + \cancel{B \cos kr}$$

spojitost vln. fce

- pro $l>0$: ... difrc ...

$$\chi \rightarrow R_l = \frac{1}{r}\chi = j_l$$

$$R_{kl}(r) \cong j_l(kr) = j_l(z)$$

alternativně algebraicky

$l \rightarrow l+1 \qquad P_+ = P_x + iP_y$

$m \rightarrow m+1$

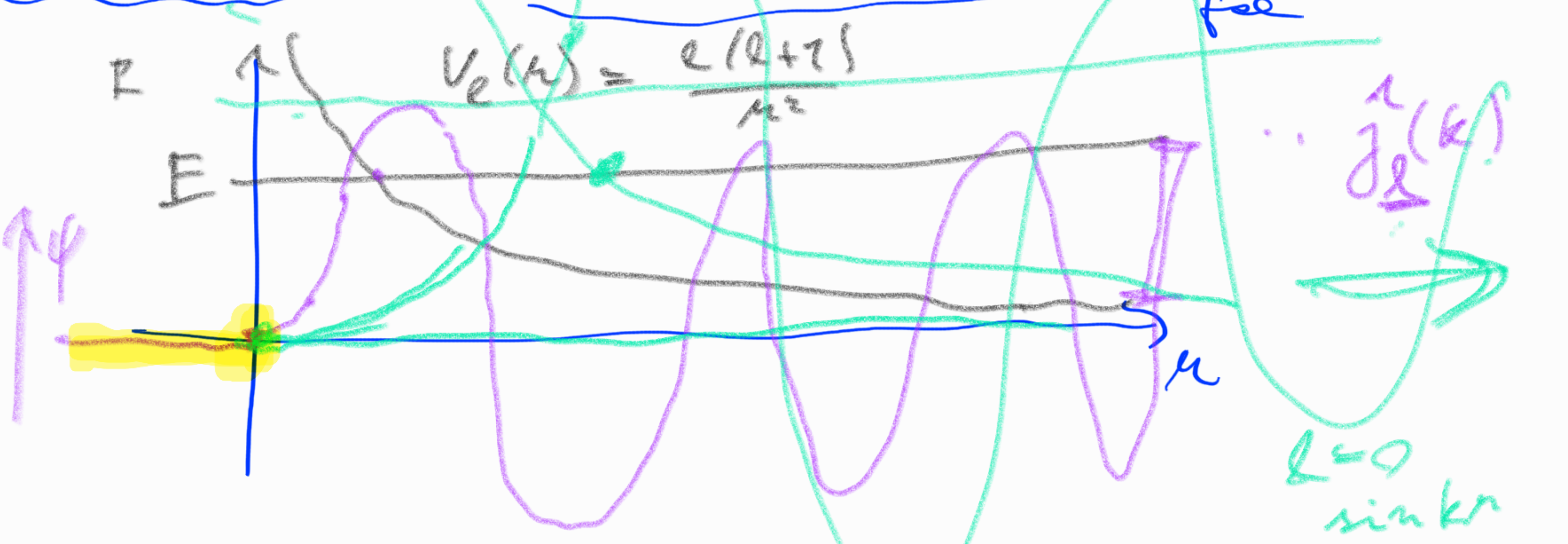
$j_l(kr)$

Cohena-Tannoudji

$$\left[\frac{d^2}{dz^2} + \frac{2}{z}\frac{d}{dz} + 1 - \frac{l(l+1)}{z^2}\right] j_l(z) = 0$$

— řešení ... sférické Besselovy fce ~ dodatek Formánkovy učebnice

$$rR = \chi \quad \ldots \quad \hat{j}_l(z) = z\, j_l(z) \quad \text{.. Riccatti-Bessel. fce}$$



$\hat{j}(kr)$ ... $\chi(r)$ .. (uSR)

z $\quad k \to 1$

z^{l+1}

$$j_l''(z) + \left[1 - \frac{l(l+1)}{z^2}\right] j_l(z) = 0 \qquad \cancel{\frac{1}{z^2}}$$

$$\frac{O(z^\alpha)}{z^\alpha} \xrightarrow[z\to 0]{} 0$$

$z \to 0$ .. $j_l(z) \sim z^\alpha + O(z^\alpha)$

$$\alpha(\alpha-1)\cancel{z^{\alpha-2}} - l(l+1)\cancel{z^{\alpha-2}} + O(\cancel{z^{\alpha-2}}) = 0$$

$l \to 0$

$$\alpha(\alpha-1) = l(l+1) \implies \boxed{\begin{array}{l}\alpha = l+1 \\ \cancel{\alpha = -l}\end{array}}$$ nefyz. řešení

$l=0$, sin

$$\hat{j}_l(z) = z^{l+1}\varphi(z)$$

P_+

$$\hat{j}_l'(z) = z^{l+1}\left(\varphi' + \frac{l+1}{z}\varphi\right)$$

$$\hat{j}_l''(z) = z^{l+1}\left(\varphi'' + \frac{2}{z}(l+1)\varphi' + \frac{l(l+1)}{z^2}\varphi\right) \qquad \frac{\cos z}{z}$$

$$\boxed{\varphi'' + \frac{2}{z}(l+1)\varphi' + \varphi = 0} \quad .. \quad l=0 \quad \boxed{\varphi_0(z) = \frac{\sin z}{z}}$$

$l \to l+1$

pozorování $\boxed{\psi = \frac{\varphi'}{z}}$ — $\boxed{\psi'' + \frac{2(l+2)}{z}\psi' + \psi = 0}$

$$\psi' = \frac{\varphi''}{z} - \frac{\varphi'}{z^2} = -\frac{1}{z}\left(\frac{2}{z}(l+1)\varphi' + \varphi\right) - \frac{\varphi'}{z^2}$$

$\psi'' =$ ------

$$\varphi_l \longrightarrow \boxed{\varphi_{l+1} = \psi(z) = \frac{1}{z}\frac{d}{dz}\varphi_l(z)}$$

$\varphi_0 \longrightarrow \forall \varphi_l$

Shrnutí:

$\boxed{\varphi \longrightarrow j}$

Závěr: $R_{kl}(r) = j_l(kl) = \frac{\hat{j}(kr)}{kr} = (kr)^l \varphi(kr)$

$\rightarrow \boxed{R_{kl}(r) = C\, j_l(kr)}$ — sférické cylindrické funkce.

$$\boxed{j_l(z) = (-1)^l z^l \left(\frac{1}{z}\frac{d}{dz}\right)^l \frac{\sin z}{z}}$$ Besselova

regulární v počátku

$$\boxed{n_l(z) = (-1)^{l+1} z^l \left(\frac{1}{z}\frac{d}{dz}\right)^l \frac{\cos z}{z}}$$ Neumannova

chování v okolí $z \to 0$

$$j_l(z) = \frac{z^l}{(2l+1)!!}$$

$N!! = N(N-2)(N-4)\cdots \,^1_2$

$$n_l(z) = \frac{(2l+1)!!}{z^{l+1}}$$

chování v $z \to \infty$

$$j_l(z) \xrightarrow[z\to\infty]{} \frac{1}{z}\sin\left(z - \frac{\pi}{2}l\right) \qquad n_l(z) = -\frac{1}{z}\cos\left(z - \frac{\pi}{2}l\right)$$

Platí: $$\boxed{\int_0^\infty j_l(kr)\, j_l(k'r)\, r^2 dr = \frac{\pi}{2k^2}\delta(k-k')}$$

-- správně normované $R_{kl}(r) = \sqrt{\frac{2}{\pi}}\, k\, j_l(kr)$

$$\langle klm | k'l'm' \rangle = \delta(k-k')\delta_{ll'}\delta_{mm'}$$