$\boxed{\text{QMI-5}}$ Bodová částice 3D – spol. vl. v. H_0, L^2, L_z

OPAKOVÁNÍ:

$$\hat H_0|klm\rangle = \frac{k^2\hbar^2}{2m}|klm\rangle$$
$$\hat L^2|klm\rangle = \hbar^2 l(l+1)|klm\rangle$$
$$\hat L_z|klm\rangle = \hbar m|klm\rangle$$

$$\langle \vec x|klm\rangle \equiv \psi_{klm}(\vec x) = R_{kl}(r)\,Y_{lm}(\theta,\varphi)$$
$$\langle klm|k'l'm'\rangle = \delta_{ll'}\delta_{mm'}\int_0^\infty R^*_{kl}R_{k'l}\, r^2\, dr = \int_0^\infty \chi^*_{kl}\chi_{k'l}\, dr$$
$$\boxed{\chi = rR}$$

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

$\rightarrow$ $R''_{kl}(r) + \frac{2}{r}R'_{kl}(r) + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_{kl} = 0$ ... $j_l(kr)$ $\quad n_l(kr)$

$\rightarrow$ $\chi''(r) + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi = 0$ ... $\hat j_l(kr)$ $\quad \hat n_l(kr)$

sférické cylindrické funkce — regulární řešení ↑ — 2. řešení ↑

Riccati-Besselovy funkce — Besselova — Neumannova

Explicitní vzorce:
$$j_l(z) \equiv (-1)^l z^l \left(\frac1z\frac{d}{dz}\right)^l \frac{\sin z}{z} \qquad \hat j_l \equiv z j_l \quad \text{"zobec. sinus"}$$
$$n_l(z) \equiv (-1)^{l+1} z^l \left(\frac1z \frac{d}{dz}\right)^l\frac{\cos z}{z} \qquad \hat n_l \equiv -z n_l \quad \text{"zobec. cosinus"}$$

regularita v počátku: $j_l(z)\simeq z^l/(2l+1)!!$ $\quad n_l(z)\simeq (2l+1)!!/z^{l+1}$ $\quad\boxed{z\to 0}$

asymptotika: $j_l \simeq \frac1z\sin\left(z-\frac\pi2 l\right)$ $\quad n_l(z)\simeq -\frac1z\cos\left(z-\frac\pi2 l\right)$ $\quad\boxed{z\to\infty}$

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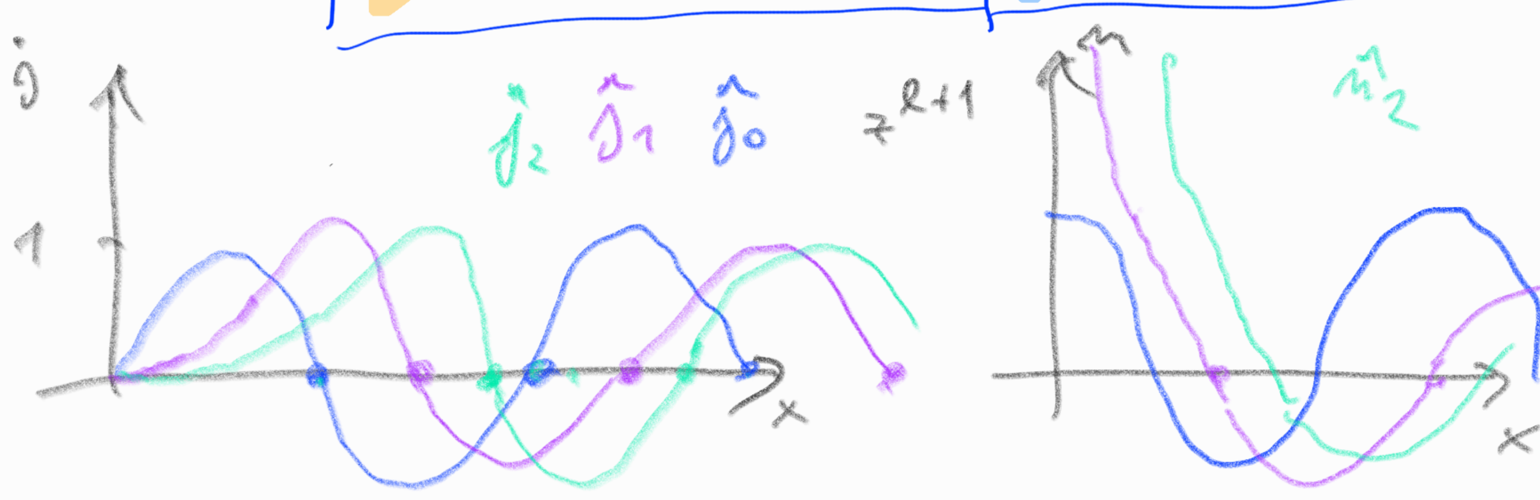
pozn: souvislost s cylindrickými (Besselovými) funkcemi
$$j_l(z) = \sqrt{\pi/2z}\, J_{l+\frac12}(z) \qquad n_l(z) = \sqrt{\pi/2z}\, N_{l+\frac12}(z)$$

Příklad .. nejnižší $l=0,1,2$:

$$j_0(z) = \frac{\sin z}{z} \qquad n_0(z) = -\frac{\cos z}{z}$$
$$j_1(z) = \frac{1}{z^2}\sin z - \frac1z\cos z \qquad n_1(z) = -\frac{1}{z^2}\cos z - \frac1z \sin z$$
$$j_2(z) = \left(\frac{3}{z^3}-\frac1z\right)\sin z - \frac{3}{z^2}\cos z \qquad n_2(z) = -\left(\frac{3}{z^3}-\frac1z\right)\cos z - \frac{3}{z^2}\sin z$$

parita (+) (−)



• chování v okolí $r \to 0$ a regularita řešení:

$$u'' + \left(k^2 - \frac{l(l+1)}{r^2}\right)u = 0 \quad \dots \quad \hat{j} \sim r^{l+1} \quad \cancel{\hat{n} \sim r^{-l}}$$

pozn. k tomu proč: jen $\hat{j}$ je fyzikální

$l = 0$ $\quad \sim kr \quad \sim 1$

$$\int_0^\infty |u|^2 \, dr = \text{konečné}$$

$$\int R^2 r^2 \, dr \qquad \psi = \frac{1}{r}\hat{u}\, Y_{lm}$$

R

$$-\frac{\hbar^2}{2m}\Delta\psi = E\psi \quad \dots \quad \frac{1}{r}$$

$$R \sim \frac{1}{r} \to \frac{1}{r^2} \quad \frac{1}{r^3} \qquad R' \quad R''$$

$\int \quad \oint$ malá sféra $r = \varepsilon$

$$\int_0^\varepsilon E\psi\, r^2 \, dr\, d\Omega \qquad \psi \sim \frac{1}{r}$$

$$4\pi E \int_0^\varepsilon r\, dr \sim \varepsilon^2$$

$$\sim \int \frac{1}{r^3} r^2 \, dr \; 4\pi$$

$$\sim \int_0^\varepsilon \frac{1}{r}\, dr \sim \ln \varepsilon \to \infty$$

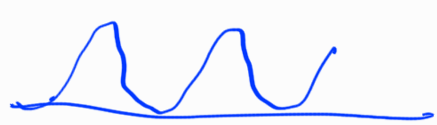
• normování:
$$\boxed{\int_0^\infty j_l(kr)\, j_l(k'r)\, r^2 \, dr = \frac{\pi}{2k^2}\,\delta(k-k')}$$

platí

Důkaz:

1) Møllerovy operátory ... izometrie ... teorie rozptylu
.. příští semestr

2) přímý důkaz:

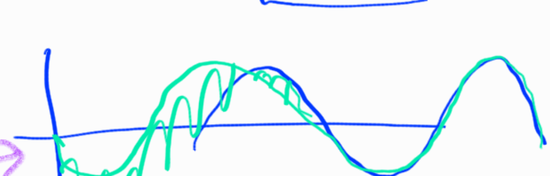


$\to \infty$

$\hat{H}_0$ .. samosdruž. $|klm\rangle$ $|k'lm\rangle$ $\qquad k = k'$, $\quad \boxed{k \neq k'}$ 0

$$j_l(kr) \to \boxed{\frac{1}{kr}\sin\left(kr - \underbrace{\frac{\pi}{2}l}_{\delta}\right)}$$

liší se o koneč. část



• δ příspěvek najdeme ze sin

$$\int_0^\infty \sin(\overbrace{kr+\delta}^{A})\sin(\overbrace{k'r+\delta}^{A'})\frac{1}{kk'}\, dr$$

$$= \frac{1}{kk'}\left(-\frac{1}{4}\right)\int_0^\infty \left(e^{iA} - e^{-iA}\right)\left(e^{iA'} - e^{-iA'}\right) dr \qquad r \to -r$$

$$\underbrace{-e^{i(A+A')} - e^{-i(A+A')}}_{\sim\,\delta(k+k') = 0} \underbrace{+ e^{i(A-A')} + e^{-i(A-A')}}_{\sim\,\delta(k-k')}$$

$k > 0 \quad k' > 0$

$$= \frac{1}{2kk'}\int_0^\infty \underbrace{\frac{1}{2}\left(e^{ir(k-k')}+e^{ir(k'-k)}\right)}_{\cos} dr = \frac{1}{4kk'}\int_{-\infty}^{\infty} \cos r(k-k')\,dr$$

$$\int i \sin r(k-k') = 0$$

$$= \frac{2\pi}{4kk'}\int_{-\infty}^{\infty} e^{2\pi i \frac{r}{2\pi}(k-k')}\frac{dr}{2\pi} = \boxed{\frac{2\pi}{4k^2}}\,\delta(k-k') \checkmark$$

$\boxed{\text{závěr:}}$ $|klm\rangle$ $\quad H_0\ L^2\ L_z$ $\quad \langle x|klm\rangle = \varphi_{klm}(\vec{x})$

$$\varphi_{klm}(\vec{x}) = \sqrt{\frac{2}{\pi}}\,k\,j_l(kr)\,Y_{lm}(\theta,\varphi)$$

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

$$E = \frac{k^2\hbar^2}{2m} \qquad \frac{2k\hbar}{2m} \cdots \frac{k\hbar}{m}$$

$$\varphi_{Elm}(\vec{x}) = \sqrt{\frac{2}{\pi}}\frac{\sqrt{mk}}{\hbar}\,j_l(kr)\,Y_{lm}(\theta,\varphi)$$

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

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5) Bodová částice ve 3D – $\hat{H}, \hat{L}^2, \hat{L}_z$ — částice ve sfér. sym. potenciálu

$$\hat{H} = \hat{H}_0 + V(\vec{x}) \qquad \underline{V(r)} \qquad r = |\vec{x}| \qquad [\hat{V}, \hat{L}_\alpha] = 0$$

$$|Elm\rangle \qquad \varphi_{Elm}(\vec{x}) = R_{El}(r)\,Y_{lm}(\theta,\varphi)$$

$$\hat{H}\varphi_{Elm} = E\varphi_{Elm}$$

(SR) $$\left(-\frac{\hbar^2}{2m}\right)\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right]R_{El} + VR_{El} = ER_{El}$$

$$\frac{2mV}{\hbar^2} = U \qquad E = \frac{\hbar^2k^2}{2m}$$

$$\rightarrow \underbrace{R''_{kl}(r) + \frac{2}{r}R'_{kl}}\ + \Big[k^2 \underbrace{- \frac{l(l+1)}{r^2} - U(r)}\Big]R_{kl} = 0$$

$$U_{eff} = U(r) + \frac{l(l+1)}{r^2}$$

$$\chi = rR$$

$$V_{eff} = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$$

$\rightarrow \quad \chi''(r) + [k^2 - \underbrace{U_{eff}(r)}] \chi(r) = 0 \qquad$ 1D SR

ODR II. ř.

• dvě řešení ... $\underline{\chi(r)\big|_{r=0} = 0}$, $\qquad$ ~~$\chi \sim 1$ jako $r \to 0$~~

E < 0 ... vázané stavy

$\boxed{0 \ldots V(r) \xrightarrow[r\to\infty]{} 0 \quad \text{BOUND}}$

požaduji $\underline{\int_0^\infty \chi^2(r)\,dr}$ konečné.

$\rightarrow$ podmínka pro výběr $\underline{E_n}$

E > 0 ... rozptylové stavy

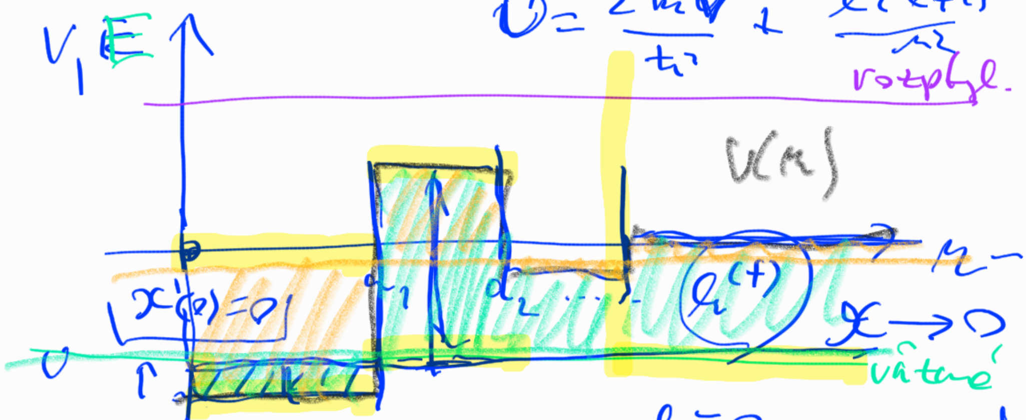
normalizace $\langle k l m | k' l' m' \rangle = \delta_{ll'}\delta_{mm'}\delta(k-k')$

$\hookrightarrow \int_0^\infty \chi_k^*(r)\,\chi_{k'}(r)\,dr = \delta(k-k')$

ANALYTICKY ŘEŠITELNÉ PŘÍPADY:

5a) Po částech konstantní potenciál

$U = \frac{2mV}{\hbar^2} + \frac{l(l+1)}{r^2}$



$l = 0$

$\chi'' + [\underbrace{k^2 - U_l}]\chi = 0$

$\rightarrow \boxed{\varkappa^2 > 0}$

$(i\varkappa)^2$

$E - V_l = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 U}{2m} = \frac{\hbar^2}{2m}(k^2 - U)$

	$l = 0$	$l > 0$
$E > V$ ...	$\sin \varkappa r \quad \cos \varkappa r$	$\hat{j}_l(\varkappa r) \quad \hat{n}_l(\varkappa r)$
$\underline{E < V}$	$e^{-\varkappa r} \quad e^{\varkappa r}$	$\varkappa r\, h_l^{(+)}(\varkappa r) \quad \boxed{\varkappa r\, h_l^{(-)}(\varkappa r)}$

$\hookrightarrow \left\{ \begin{array}{l} \hat{j}_l(i\varkappa r) \longrightarrow \sin(i\varkappa r + \delta) \\ \hat{n}_l(\underline{i\varkappa r}) \longrightarrow \cos(i\varkappa r + \delta) \end{array} \right\} e^{\pm i \underline{Arg}} = \cos \ldots$

Hankelovy fce $\underline{h_l^{(\pm)}(z) = j_l(z) \pm i\,n_l(z) \xrightarrow[z\to\infty]{} (\mp i)^{l+1}\frac{1}{z}e^{\pm iz}}$

$h_\ell^{(\pm)}(\varkappa r) \underset{r\to\infty}{\sim} e^{\pm \varkappa r}$ ... okraj. podm.

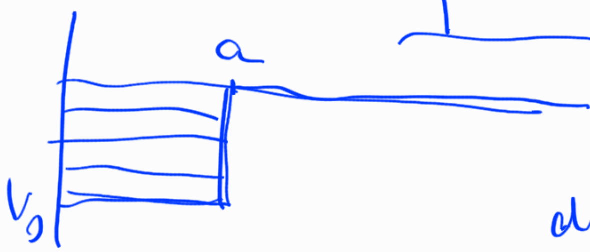
$\to \chi(0)=0$

$\to$ pro $E<0$ ... $-\frac{\varkappa^2\hbar^2}{2m}$, $k=i\varkappa$

$\chi(r\to\infty) = C\cdot h_\ell^{(+)}(\varkappa r)$

$\underline{z = kr = i\varkappa r}$

$$h^{(+)} \sim \boxed{e^{+iz}} = e^{+i i \varkappa r} = \boxed{e^{-\varkappa r}}$$



diskrét.

$$\boxed{1 = \int \psi^* \psi \, d^3x}$$

$$\boxed{\psi \sim \frac{1}{x^{3/2}}}$$

spojité $\underline{[\delta(\lambda-\lambda')]}$ ... $\frac{1}{[\lambda]} = \int \psi_\lambda^* \psi_{\lambda'} \, d^3x$

$[\lambda]$ $\qquad \frac{1}{[\lambda][x^{3/2}]}$

$|E\ell m\rangle$

$|k\ell m\rangle$