přednáška ÚDKM 27.2.2020

$10^{40} - 12^{10}$, M1

(1) MOTIVACE

Schrödinger navrhl (192) $\hat{H}\Psi = E\Psi$

hamiltonián = operátor energie

Ψ = vlnová fce popisující náš systém

$\hat{H} = \frac{\hat{p}^2}{2} - \frac{1}{\hat{r}}$ ← v atomových jednotkách (bude podrobněji na přednášce)

měříme jeho vlastní hodnoty = energie

v souřadnicové repre (podrobněji na přednášce)

$\hat{\vec{r}} \to \vec{r}$

$\hat{\vec{p}} \to -i\nabla$

pro (→ tady; zmínit tady) hamiltonián $\hat{H} = \frac{\hat{p}^2}{2} + V(\hat{r})$

(potenciál závislý pouze na r) = sférický potenciál

existuje ÚMKO = úplná množina komutujících operátorů

$\{\hat{H}, \hat{L}^2, \hat{L}_z\}$

náš ham.

$\hat{\vec{L}}$ = operátor momentu hybnosti

→ $\hat{L}^2$ → kvadrát $\hat{\vec{L}}$

→ $\hat{L}_z$ → projekce momentu hybnosti do směru osy z

$[H, L^2] = 0$

$[H, L_z] = 0$

$[L^2, L_z] = 0$

komutátor dvou operátorů

$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

~~sférický potenciál → výhodné přejít do sférických souřadnic~~

⇒ můžeme zvolit společnou bázi vl. ~~vektorů~~ funkcí $\Psi_{n,l,m}(\vec{r})$

$\hat{H}\Psi_{n,l,m}(\vec{r}) = -\frac{1}{2n^2}\Psi_{n,l,m}$

$\hat{L}^2\Psi_{n,l,m}(\vec{r}) = l(l+1)\Psi_{n,l,m}(\vec{r})$ $l = 0, \dots, n-1$

$\hat{L}_z\Psi_{n,l,m}(\vec{r}) = m\Psi_{n,l,m}(\vec{r})$ $m = -l, \dots, l$

(2)

sférická symetrie → výhodné přejít do sférických souřadnic:

$x_i = r n_i$

r: radiální souř.; n_i: úhlové souř., jednotkový směrový vektor

$x = r\sin\theta\cos\varphi$

$y = r\sin\theta\sin\varphi$

$z = r\cos\theta$

(2)

$x_i = r n_i$

$$p_i = -i\frac{\partial}{\partial x_i} = -i\left(\frac{\partial r}{\partial x_i}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x_i}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x_i}\frac{\partial}{\partial \varphi}\right)$$

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\}$$ ⇝ chceme vyjádřit r, θ, φ:

$$x^2+y^2+z^2 = r^2\sin^2\theta\cos^2\varphi + r^2\sin^2\theta\sin^2\varphi + r^2\cos^2\theta = r^2$$

$$x^2+y^2 = r^2\sin^2\theta(\cos^2\varphi+\sin^2\varphi) = \frac{z^2}{\cos^2\theta}\sin^2\theta$$

$$\frac{x}{y} = \frac{r\sin\theta\cos\varphi}{r\sin\theta\sin\varphi} \qquad \frac{y}{x} = \frac{\sin\varphi}{\cos\varphi}$$

$$\Rightarrow \quad r = \sqrt{x^2+y^2+z^2}, \quad \theta = \operatorname{arctg}\frac{\sqrt{x^2+y^2}}{z}, \quad \varphi = \operatorname{arctg}\frac{y}{x}$$

$$p_i = -i\left(\frac{\partial r}{\partial x_i}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x_i}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x_i}\frac{\partial}{\partial \varphi}\right) = -i\frac{\partial}{\partial x_i}$$

$$\frac{\partial r}{\partial x_i} = \frac{x_i}{r} \; : \; \frac{\partial}{\partial x}\left(\sqrt{x^2+y^2+z^2}\right) = \frac{1}{2r}\cdot 2x = \frac{x}{r} = \frac{r\sin\theta\cos\varphi}{r} = \sin\theta\cos\varphi \text{ atd.}$$

$$\frac{\partial \theta}{\partial x_i} = \; : \; \frac{\partial \theta}{\partial x} = \frac{\partial}{\partial x}\left(\operatorname{arctg}\frac{\sqrt{x^2+y^2}}{z}\right) = \frac{1}{1+\frac{x^2+y^2}{z^2}}\cdot\frac{1}{z}\frac{1}{2\sqrt{x^2+y^2}}\cdot 2x \qquad (\operatorname{arctg} x)' = \frac{1}{1+x^2}$$

$$= \frac{z\cdot x}{\underbrace{(x^2+y^2+z^2)}_{r^2}\sqrt{x^2+y^2}} = \frac{r\cos\theta\, r\sin\theta\cos\varphi}{r^2\; r\sin\theta} = \frac{1}{r}\cos\theta\cos\varphi$$

$$\frac{\partial \theta}{\partial y} = \frac{\partial}{\partial y}\left(\operatorname{arctg}\frac{\sqrt{x^2+y^2}}{z}\right) = \frac{zy}{(x^2+y^2+z^2)\sqrt{x^2+y^2}} = \frac{r\cos\theta\; r\sin\theta\sin\varphi}{r^2\; r\sin\theta} = \frac{1}{r}\cos\theta\sin\varphi$$

$$\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left(\operatorname{arctg}\frac{\sqrt{x^2+y^2}}{z}\right) = \frac{z^2}{r^2}\cdot\sqrt{x^2+y^2}\cdot\frac{-1}{z^2} = -\frac{r\sin\theta}{r^2} = -\frac{1}{r}\sin\theta$$

$$\frac{\partial \varphi}{\partial x_i} = \; : \; \frac{\partial \varphi}{\partial x} = \frac{\partial}{\partial x}\left(\operatorname{arctg}\frac{y}{x}\right) = \frac{1}{1+(\frac{y}{x})^2}\cdot\frac{-y}{x^2} = -\frac{r\sin\theta\sin\varphi}{r^2\sin^2\theta} = -\frac{\sin\varphi}{r\sin\theta}$$

$$\frac{\partial \varphi}{\partial y} = \frac{\partial}{\partial y}\left(\operatorname{arctg}\frac{y}{x}\right) = \frac{1}{1+(\frac{y}{x})^2}\cdot\frac{1}{x} = \frac{x}{x^2+y^2} = \frac{r\cos\theta\sin\varphi}{r^2(\cos^2\theta\sin^2\varphi+\sin^2\theta\sin^2\varphi)} = \frac{\cos\varphi}{r\sin\theta}$$

$$\frac{\partial \varphi}{\partial z} = 0$$

$$\boxed{\frac{\partial}{\partial x_i} = n_i\frac{\partial}{\partial r} + \frac{\nabla^n_i}{r}}$$ ⟶ tzn. $p_i = -i\frac{\partial}{\partial x_i} = -i\left(n_i\frac{\partial}{\partial r} + \frac{\nabla^n}{r}\right)$

$\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ směrový vektor

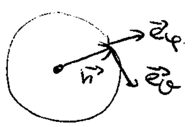
$\nabla^n = \vec{e}_\theta\frac{\partial}{\partial\theta} + \frac{\vec{e}_\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}$ ⇝ obsahuje všechny úhlové derivace

$\vec{e}_\theta = (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta)$

$\vec{e}_\varphi = (-\sin\varphi, \cos\varphi, 0)$

navzájem kolmé vektory

⇝ můžou si doma ověřit



③ $\boxed{\vec{n}\cdot\nabla^n = 0}$:

$$\vec{n} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$$

$$\nabla^n = \vec{e}_\vartheta \frac{\partial}{\partial\vartheta} + \frac{\vec{e}_\varphi}{\sin\vartheta}\frac{\partial}{\partial\varphi}$$

$$\vec{e}_\vartheta = (\cos\vartheta\cos\varphi, \cos\vartheta\sin\varphi, -\sin\vartheta)$$
$$\vec{e}_\varphi = (-\sin\varphi, \cos\varphi, 0)$$

$$\left.\begin{array}{l}\vec{n}\cdot\vec{e}_\vartheta = 0\\ \vec{n}\cdot\vec{e}_\varphi = 0\end{array}\right\} \Rightarrow \underline{\vec{n}\cdot\nabla^n = 0}$$

④ $\boxed{\left[\frac{\partial}{\partial x_i}, x_j\right] = \delta_{ij}}$

obecně: $\left[\frac{\partial}{\partial x}, f(x)\right] = \frac{\partial f}{\partial x}$: $[A,B] = AB - BA$

→ představme si ještě jednu fci g, na kt. operátory působí:

$$\left[\frac{\partial}{\partial x}, f(x)\right]g = \frac{\partial}{\partial x}(f(x)g) - f(x)\frac{\partial}{\partial x}g$$
$$= \frac{\partial f(x)}{\partial x}g + f(x)\frac{\partial g}{\partial x} - f(x)\frac{\partial}{\partial x}g$$
$$= \frac{\partial f(x)}{\partial x}g \Rightarrow \underline{\left[\frac{\partial}{\partial x}, f(x)\right] = \frac{\partial f(x)}{\partial x}}$$

$$\frac{\partial}{\partial x_i}(x_j f) - x_j\frac{\partial}{\partial x_i}f =$$
$$= \underbrace{\frac{\partial x_j}{\partial x_i}}_{\delta_{ij}} f + x_j\frac{\partial f}{\partial x_i} - x_j\frac{\partial f}{\partial x_i} = \delta_{ij} f$$

⑤ $[\underbrace{n_i\frac{\partial}{\partial r} + \frac{D_i^n}{r}}_{p_i}, \underbrace{r n_j}_{x_j}] = \delta_{ij} \Longrightarrow \boxed{[D_i^n, n_j] = \delta_{ij} - n_i n_j}$

$$\left[n_i\frac{\partial}{\partial r} + \frac{D_i^n}{r}, rn_j\right] = \underbrace{\left[n_i\frac{\partial}{\partial r}, rn_j\right]}_{\downarrow} + \underbrace{\left[\frac{D_i^n}{r}, rn_j\right]}_{=[D_i^n, n_j]} = n_i n_j + [D_i^n, n_j] = \delta_{ij} \rightarrow \underline{[D_i^n, n_j] = \delta_{ij} - n_i n_j}$$

$$n_i\frac{\partial}{\partial r}(rn_j f) - rn_j n_i\frac{\partial}{\partial r}f$$
$$n_i n_j f + n_i r n_j\frac{\partial f}{\partial r} - rn_j n_i\frac{\partial f}{\partial r}$$

$$\Rightarrow \boxed{[D_i^n, n_i] = \delta_{ii} - n_i n_i = 3 - 1 = 2}$$

$$\Rightarrow \quad = D_i^n(n_i f) - n_i D_i^n f = \boxed{D_i^n n_i = 2}$$

⑥ zavedeme moment hybnosti: (jako v klasické mechanice a ostatní zkoumejme) $\rightsquigarrow \vec{L} = \vec{r}\times\vec{p}$

$$\hat{L}_i = \varepsilon_{ijk}\hat{x}_j\hat{p}_k \longrightarrow \hat{L}_i = -i\varepsilon_{ijk}x_j\frac{\partial}{\partial x_k}$$
$$\hat{x}_j \to x_j$$
$$\hat{p}_k \to -i\frac{\partial}{\partial x_k}$$

$$\underline{\underline{L_i}} = \varepsilon_{ijk}x_j p_k \to -i\varepsilon_{ijk}x_j\frac{\partial}{\partial x_k}$$
$$= -i\varepsilon_{ijk}rn_j\left(n_k\frac{\partial}{\partial r} + \frac{D_k^n}{r}\right)$$
$$= \underbrace{-i\varepsilon_{ijk}rn_j n_k\frac{\partial}{\partial r}}_{A\,\cdot\,S\;=0} - i\varepsilon_{ijk}rn_j\frac{D_k^n}{r}$$
$$= \underline{\underline{-i\varepsilon_{ijk}n_j D_k^n}}$$

! pouze úhlová závislost, radiální ne!

(7) $\boxed{[\hat{L}_i,\hat{L}_j] = i\varepsilon_{ijk}\hat{L}_k}$ což plyne z $[p_i,x_j] = -i\delta_{ij}$ $\quad \hat{L}_i = \varepsilon_{ijk}x_j p_k$

$$[\hat{L}_i,\hat{L}_j] = [\varepsilon_{ipq}x_p p_q, \varepsilon_{jmn}x_m p_n] =$$

$$= +\varepsilon_{ipq}\varepsilon_{jmn}[x_p p_q, x_m p_n] =$$

$$[AB,C] = A[B,C] + [A,C]B$$ ← důkaz roznásobením (je to jako derivování)

$$= +\varepsilon_{ipq}\varepsilon_{jmn}\{x_p[p_q,x_m p_n] + [x_p,x_m p_n]p_q\}$$

$$[p_q,p_n]=0 \qquad [x_p,x_m]=0$$

$$= +\varepsilon_{ipq}\varepsilon_{jmn}\{x_p \underbrace{[p_q,x_m]}_{=-i\delta_{qm}} p_n + x_m \underbrace{[x_p,p_n]}_{=i\delta_{pn}} p_q\}$$

$$= -i(\underbrace{\varepsilon_{ipm}\varepsilon_{jmn}}_{=\varepsilon_{mip}\varepsilon_{mnj}} x_p p_n + \underbrace{\varepsilon_{ipq}\varepsilon_{jmp}}_{=\varepsilon_{pqi}\varepsilon_{pjm}} x_m p_q)$$

$$\varepsilon_{mip}\varepsilon_{mnj} = \delta_{in}\delta_{pj} - \delta_{ij}\delta_{pn} \qquad \varepsilon_{pqi}\varepsilon_{pjm} = \delta_{qj}\delta_{im} - \delta_{ij}\delta_{qm}$$

$$= -i(x_j p_i - \delta_{ij}x_p p_p - x_i p_j + \delta_{ij} x_q p_q)$$

pouze sčítací indexy → $q = p$

$$= +i(x_i p_j - x_j p_i)$$

$$i\varepsilon_{ijk}L_k = i\varepsilon_{ijk}\varepsilon_{kmn}x_m p_n = i\varepsilon_{kij}\varepsilon_{kmn}x_m p_n =$$

$$= i(\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})x_m p_n$$

$$= i(x_i p_j - x_j p_i)$$

$$\Rightarrow \underline{\underline{[\hat{L}_i,\hat{L}_j] = i\varepsilon_{ijk}\hat{L}_k}}$$

(8) $[\hat{L}_i,\hat{L}_j] = i\varepsilon_{ijk}\hat{L}_k \Rightarrow \boxed{[\hat{L}_k,\hat{L}^2] = 0}$ $\quad \hat{L}^2$ komutuje s lib. složkou $\hat{L}_k$

$$[L_k,L^2] = [L_k,L_m L_m] = L_m[L_k,L_m] + [L_k,L_m]L_m =$$

$$\uparrow$$

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

$$= L_m i\varepsilon_{kmn}L_n + i\varepsilon_{kmn}L_n L_m$$

$$= i\underbrace{\varepsilon_{kmn}}_{A,\ m\leftrightarrow n}\underbrace{(L_m L_n + L_n L_m)}_{S,\ m\leftrightarrow n} = \underline{\underline{0}}$$

(9) $\underline{D^2} = \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i} = \left(n_i\frac{\partial}{\partial r} + \frac{D_i^n}{r}\right)\left(n_i\frac{\partial}{\partial r} + \frac{D_i^n}{r}\right) =$

$$= n_i\frac{\partial}{\partial r}\left(n_i\frac{\partial}{\partial r}\right) + n_i\frac{\partial}{\partial r}\left(\frac{D_i^n}{r}\right) + \frac{D_i^n}{r}n_i\frac{\partial}{\partial r} + \frac{D_i^n}{r}\frac{D_i^n}{r}$$

$$\underbrace{n_i n_i}_{=1}\frac{\partial^2}{\partial r^2} = \frac{\partial^2}{\partial r^2} \qquad \underbrace{n_i D_i^n}_{=0\ \text{(výše)}}\left(\frac{-1}{r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) \qquad \underbrace{D_i^n n_i}_{=2\ \text{(výše)}}\frac{1}{r}\frac{\partial}{\partial r} \qquad = \frac{1}{r^2}(D_i^n)^2$$

$$= \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(D^n)^2}{r^2}$$

$$\boxed{D^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(D^n)^2}{r^2}}$$

$\underline{\hat{L}^2} = L_i L_i = \varepsilon_{ijk} x_j p_k \varepsilon_{ipq} x_p p_q$

~~$x_j = r n_j$, $p_k = -i D_k^n$~~

~~$= \varepsilon_{ijk}\varepsilon_{imn} r n_j (-i) D_k^n r n_p (-i) D_q^n$~~

~~$= (\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) r^2 n_j D_k^n n_p D_q^n$~~

$L_i = \varepsilon_{ijk} x_j p_k = \dots = -i\varepsilon_{ijk} n_j D_k^n$ (ukázali jsme dříve)

$$= (-i)\varepsilon_{ijk} n_j D_k^n (-i)\varepsilon_{ipq} n_p D_q^n$$

$$= -(\delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp}) n_j D_k^n n_p D_q^n$$

$$= -(n_p D_q^n n_p D_q^n - n_q \underbrace{D_p^n n_p}_{=2} D_q^n)$$

$$D_q^n n_p = n_p D_q^n + \delta_{qp} - n_q n_p$$

$$[D_q^n, n_p] = D_q^n n_p - n_p D_q^n = \delta_{qp} - n_q n_p$$

$$= -\left[n_p(n_p D_q^n + \delta_{qp} - n_q n_p) D_q^n - 2\underbrace{n_q D_q^n}_{=0}\right]$$

$$= -\underbrace{n_p n_p}_{=1} D_q^n D_q^n - \underbrace{n_p D_p^n}_{=0} + \underbrace{n_p n_q n_p D_q^n}_{=1\ \ =0}$$

$$= -D_q^n D_q^n = \underline{-(D^n)^2}$$

$$\Rightarrow \boxed{\hat{L}^2 = -(D^n)^2}$$

(10) vrátíme se zpátky k našemu hamiltoniánu se sférickým potenciálem

$$\underline{\hat{H}} = \frac{\hat{p}^2}{2} + V(\hat{r}) = \frac{-D^2}{2} + V(r) = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(D^n)^2}{r^2}\right) + V(r)$$

$\hat{p} \to -i\hbar\frac{\partial}{\partial x_i}$, $\hat{x}_i \to x_i$

$$= -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L^2}{r^2}\right) + V(r)$$

$\{H, L^2, L\}$ ÚMKO:

$[\hat{L}_i, \hat{L}^2] = 0$ jsme už ukázali

$[H, L^2] = 0$

$[L_i, H] = 0$

} vidíme (protože)

(11) zavedeme radiální hybnost $p_r = -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$

$$\Rightarrow p_r^2 = -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)(-i)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$= -\left(\frac{\partial^2}{\partial r^2} - \frac{1}{r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\right)$$

$$= -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$$

$$\Rightarrow \vec{p}\cdot\vec{p} = -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(\ldots)^2}{r^2}\right)$$

$$= p_r^2 + \frac{L^2}{r^2}$$

$$\Rightarrow H = \frac{\vec{p}\cdot\vec{p}}{2} + V(r) = \frac{p_r^2}{2} + \frac{L^2}{2r^2} + V(r)$$

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až sem máme určitě dojít

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(12) $H = \frac{p_r^2}{2} + \frac{L^2}{2r^2} + V(r)$

protože máme ÚMKO $\{H, L^2, L_z\}$

$H\psi = E\psi$

vln. fci můžeme charakterizovat 3 QČ (jak se učí na střední...)

$$\left(\frac{p_r^2}{2} + \frac{L^2}{2r^2} + V(r)\right)\psi_{n,l,m} = E_{n,l}\psi_{n,l,m}$$

energie obecně závisí na n a l

* na m nezávisí, protože m se nevyskytuje v $\hat{H}$
* speciálně pro coulombovský potenciál $V(r) \propto -\frac{1}{r}$ (a jen pro něj) energie závisí pouze na n

(stačí trochu jiný potenciál – i třeba jen relativistické korekce – a energie už závisí na l)

$E = -\frac{1}{2n^2}$

$$H\psi_{n,l,m} = E_{n,l}\psi_{n,l,m}$$

$$L^2\psi_{n,l,m} = l(l+1)\psi_{n,l,m}$$

$$L_z\psi_{n,l,m} = m\psi_{n,l,m}$$

$$\Rightarrow \left(\frac{p_r^2}{2} + \frac{l(l+1)}{2r^2} + V(r)\right)\psi_{n,l,m}(r,\theta,\varphi) = E_{n,l}\psi_{n,l,m}(r,\theta,\varphi)$$

vlnovou fci lze separovat: $\psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)\, Y_{lm}(\hat{r})$

$R_{n,l}(r)$ – radiální část; $Y_{lm}(\hat{r})$ – úhlová část $\Rightarrow$ sférické harmonity

$$\left[\frac{p_r^2}{2} + \frac{l(l+1)}{2r^2} + V(r)\right]R_{n,l} = E_{n,l}R_{n,l}$$

$$L^2 Y_{lm} = l(l+1)Y_{lm}$$

$$L_z Y_{lm} = m Y_{lm}$$

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konec první části na stihnutí

pokud zbyde čas:

(13) $$[L_i, n_j] = i\,\varepsilon_{ijk} n_k$$

$$\underline{[L_i, n_j]} = [i\,\varepsilon_{ipq} n_p D^n_q, n_j] = -i\,\varepsilon_{ipq}[n_p D^n_q, n_j] =$$

$$= -i\,\varepsilon_{ipq} n_p \underbrace{[D^n_q, n_j]}_{\delta_{qj} - n_q n_j}$$

$$= -i\,\varepsilon_{ipq} n_p \delta_{qj} + i\,\varepsilon_{ipq} n_p n_q n_j$$

$p \leftrightarrow q$: A; $p \leftrightarrow q$: S $\Rightarrow 0$

$$= -i\,\varepsilon_{ipj} n_p$$

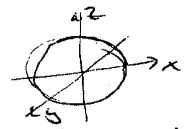
$$= \underline{i\,\varepsilon_{ijk} n_k} \qquad \varepsilon_{ipj} = -\varepsilon_{ijp}$$

(14) $$[L^2, n_j] = -2(D^{(n)}_j - n_j)$$

$$\underline{[L^2, n_j]} = [-(D^n_k)^2, n_j] = [-D^n_k D^n_k, n_j] = -D^n_k \underbrace{[D^n_k, n_j]}_{=\delta_{kj} - n_k n_j} - \underbrace{[D^n_k, n_j]}_{=\delta_{kj} - n_k n_j} D^n_k =$$

$$= -D^n_j + \underbrace{D^n_k n_k}_{=2} n_j - D^n_j + \underbrace{n_k n_j D^n_k}_{= n_j (n_k D^n_k) = 0}$$

$$= \underline{-2(D^n_j - n_j)}$$



(15) jak vypadají kulové fce $Y_{lm}(\vec{n})$?

→ začneme od $Y_{00}(\vec{n})$: → žádná úhlová závislost, jen konstanta → s-orbital – tak, jak ho známe ze středoškolské chemie

$$L^2 Y_{00}(\vec{n}) = 0$$

$$L_z Y_{00}(\vec{n}) = 0$$

určíme z normalizace

$$\int |Y_{00}|^2 \, d\Omega = 1$$

$d\Omega = \sin\vartheta \, d\vartheta \, d\varphi$

$$|Y_{00}|^2 \int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} d\varphi = |Y_{00}|^2 \cdot 2 \cdot 2\pi = 4\pi |Y_{00}|^2 \overset{!}{=} 1$$

$$\Rightarrow \underline{Y_{00} = \frac{1}{\sqrt{4\pi}}}$$

→ a ukážeme, že z Y_{00} můžeme získat další orbitaly (p, d, ...)

($l=1$, $m_z = -1, 0, 1$; $l=2$, $m_z = -2, -1, 0, 1, 2$)

↳ použijeme k tomu komutátor $[L^2, n_j] = 2(n_j - D^n_j)$ ← operátorová rovnost, musí platit, i když zapůsobíme na fci

$$[L^2, n_j]\, Y_{00} = 2(n_j - D^n_j)\, Y_{00}$$

$$(L^2 n_j - n_j \underbrace{L^2) Y_{00}}_{=0} = 2(n_j - \underbrace{D^n_j) Y_{00}}_{=0}$$ (protože není žádná úhlová závislost)

$$L^2 (n_j Y_{00}) = 2 (n_j Y_{00}) = 1(1+1)(n_j Y_{00})$$

nová fce s $l=1$ → $j = x, y, z$ ⇒ $\underline{p_x, p_y, p_z \text{ orbital}}$

(vl. fce L^2, ale ne L_z)

a podobně můžeme získat d-orbitaly:

zapůsobíme zleva komutátorem $[L^2, n_j]$:

$$[L^2, n_j]\, n_k Y_{00} = 2(n_j - D_j^n)\, n_k Y_{00}$$

$$(L^2 n_j - n_j L^2)\, n_k Y_{00} = 2 n_j n_k Y_{00} - 2 D_j^n n_k Y_{00} \quad \to n_k D_j^n + \delta_{kj} - n_k n_j, \quad D_j^n Y_{00} = 0$$

$\Rightarrow 2$

$$L^2 n_j n_k Y_{00} - 2 n_j n_k Y_{00} = 2 n_j n_k Y_{00} - 2(\delta_{kj} - n_k n_j) Y_{00}$$

~~$/ -\frac{1}{3}\delta_{jk} Y_{00}$ a na obě strany~~

$$L^2 \left(n_j n_k - \tfrac{1}{3}\delta_{jk}\right) Y_{00} = 6\left(n_j n_k - \tfrac{1}{3}\delta_{kj}\right) Y_{00}$$

tohle jsme přidali ⇐ můžeme, protože $L^2 \delta_{jk} Y_{00} = \delta_{jk} L^2 Y_{00} = \delta_{jk}\, 0 = 0$

$6 = 2(2+1) \Rightarrow \left(n_j n_k - \frac{1}{3}\delta_{kj}\right) Y_{00}$ jsou vl. fce L^2 s $l = 2$

↳ d-orbitaly

(opět chemické, ne vl. fce L_z)

vlastní fce L_z můžeme dostat podobně:

(16) $\vec{n} = (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta)$ (n_1, n_2, n_3)

zavedeme snižovací a zvyšovací operátory ("ladder operators")

$$n_\pm = n_1 \pm i n_2 = \sin\theta\cos\varphi \pm i \sin\theta\sin\varphi$$
$$= \sin\theta(\cos\varphi \pm i\sin\varphi)$$
$$= \sin\theta\, e^{\pm i\varphi}$$

$$n_3 = \cos\theta$$

($n_1 = n_x$, $n_2 = n_y$, $n_3 = n_z$)

$[L_i, n_j] = i\varepsilon_{ijk} n_k \Rightarrow$
- $[L_z, n_z] = 0$
- $[L_z, n_\pm] = [L_z, n_x \pm i n_y] = [L_z, n_x] \pm i [L_z, n_y]$

(viz dříve)

$$= i\varepsilon_{zxy} n_y \pm i(i\varepsilon_{zyx}) n_x$$

($\varepsilon_{zxy} = +1$, $\varepsilon_{zyx} = -1$)

$$= \pm(n_x \pm i n_y) = \pm n_\pm$$

a opět působíme op. rovnosti na Y_{00}:

$$[L_z, n_z] Y_{00} = 0 \qquad [L_z, n_\pm] Y_{00} = \pm n_\pm Y_{0,0}$$

$$L_z n_z Y_{00} = 0 \qquad (L_z n_\pm - n_\pm L_z) Y_{00} = \pm n_\pm Y_{00}$$

($L_z Y_{00} = 0$)

$$L_z (n_\pm Y_{00}) = \pm (n_\pm Y_{00})$$

$$\Rightarrow Y_{10} \propto n_z Y_{00}$$
$$Y_{1,\pm 1} \propto n_\pm Y_{00}$$

až na konst. → z normalizace $\int d\Omega\, |Y_{l,m}|^2 = 1$

$$\Rightarrow Y_{10} = \sqrt{\frac{3}{4\pi}}\, n_z = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{1,\pm 1} = (\pm)\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{\pm i\varphi}$$