Plán: de Broglie — UK, e^-, m & p^+

UKM 2023-I-1

- operátory, fce, matice op, vektory
  - lineární
- akce — $\cos\phi$, $\sin\phi$, $\frac{d}{d\phi}$ jako příklad

DÚ
- bit
- bit
- komutátor < std, matice

VZTAHY

světlo

$E = \hbar\omega$

$E = pc$

$p = \frac{h}{\lambda}$

částice – volné $E = \frac{1}{2}mv^2$; $p = mv = \sqrt{2Em}$, $v = \sqrt{\frac{2E}{m}}$

$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$ $\qquad \lambda = \frac{h}{mv}$

← 80kg, $10\,m\,s^{-1}$

$\lambda = \frac{h}{p} = \frac{6.626 \cdot 10^{-34}}{m \cdot v} = \frac{6.626 \cdot 10^{-34}}{80 \cdot 10} \approx \frac{6.626 \cdot 10^{-34}}{10^3} \approx 7 \cdot 10^{-37}\,m$

O_2 in air $500\,m\,s^{-1}$ (air temp)

$\lambda = \frac{h}{p} = \frac{6.626 \cdot 10^{-34}}{53 \cdot 10^{-27} \cdot 500} = \frac{6.626 \cdot 10^{-7}}{53 \cdot 500} \doteq 2.5 \cdot 10^{-11}\,m$

$m(O_2) = 32 \cdot 1.66 \cdot 10^{-27}\,kg = 53.12 \cdot 10^{-27}$

$C_{60} = \frac{6.626 \cdot 10^{-34}}{200 \cdot 60 \cdot 12 \cdot 1.66 \cdot 10^{-27}} = \frac{6.626 \cdot 10^{-10}}{144 \cdot 1.66 \cdot 3}$

$\lambda = \frac{h}{\sqrt{2mE}} = \frac{2\pi\hbar}{\sqrt{2mE}}$ atomic units $m_e = \hbar = q_e = 1$

1) e^-, $E = 1\,eV = \frac{1}{27.2114}\,Ha$

$\lambda = \frac{2\pi\hbar}{\sqrt{2mE}} \xrightarrow{a.u.} = \frac{2\pi}{\sqrt{2Em_r}} = \frac{2\pi \cdot \sqrt{27.2114}}{\sqrt{2}} = 2\pi\sqrt{13.6} = 23\,[\mathrm{Bohr}]$

m_r ← relative weight to e^-

$E = \frac{1}{2}\,Ha$

$\lambda = \frac{2\pi}{\sqrt{2E}} = \frac{2\pi}{\sqrt{2 \cdot \frac{1}{2}}} = 2\pi\,[\mathrm{Bohr}]$ & p^+ e^-

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$E = \frac{3}{2}k_B T$

$\lambda = \frac{2\pi\hbar}{\sqrt{2m\frac{3}{2}k_B T}} = \frac{2\pi\hbar}{\sqrt{3mk_B T}} \xrightarrow{a.u.} \frac{2\pi}{\sqrt{3\mu T \, 3.1685 \cdot 10^{-6}}}$

$\doteq 2038 \frac{1}{\sqrt{\mu T}}$

- $\lambda = \frac{2038}{\sqrt{\mu T}}$ [Bohr]

- p^+: $m_p = 1836\, m_e$

  $T = 20K$ $\rightarrow \lambda = \frac{2038}{\sqrt{1836 \cdot 20}} \approx 10.6$ B ~ 5 Å

  $T = 300K$ $\rightarrow \lambda = \frac{2038}{\sqrt{1836 \cdot 20}} \approx 2.75$ B ~ 1.45 Å

  d^+: $m_d = 3670\, m_e$

  $T = 300K$ $\rightarrow \lambda = 1.94$ B ~ 1.03 Å

Operátory, [fce, lin. algebra]

Lineární: $\hat{A}(f+g) = \hat{A}(f) + \hat{A}(g)$

$\hat{A}(cf) = c\hat{A}(f)$

- $\hat{A} = \frac{d}{dx}$ $\rightarrow \frac{d}{dx}(f+g) = \frac{df}{dx} + \frac{dg}{dx} = \hat{A}(f) + \hat{A}(g)$

$\hat{A}c$ $\rightarrow \frac{d}{dx}(cf) = c\frac{df}{dx} = c\hat{A}(f)$

$\hat{A}: f \mapsto \frac{1}{f}$ $\rightarrow \hat{A}(f+g) = \frac{1}{f+g}$ $\times$

- operátory $\hat{x}$ a $\frac{\hat{d}}{dx}$: složité operátory i) zjednodušení pomocí testovací fce
  ii) zjednodušení pomocí [,]

$\hat{A} = \hat{x}$ $\quad \hat{B} = \frac{\hat{d}}{dx}$

$\hookrightarrow f \to xf \quad f \to f'$

$\hat{A}\hat{B}f = \hat{x}\frac{\hat{d}}{dx}f = \hat{x}\cdot f' = xf' = \left(x\cdot\frac{d}{dx}\right)f \Rightarrow \hat{C} = \hat{A}\hat{B} = \hat{x}\frac{\hat{d}}{dx}$

$\hat{B}\hat{A}f = \frac{\hat{d}}{dx}\hat{x}f = \frac{\hat{d}}{dx}xf = f + xf' = \left(1 + x\frac{d}{dx}\right)f \Rightarrow \hat{D} = \hat{B}\hat{A} = \frac{\hat{d}}{dx}\hat{x} = \left(\hat{1} + \hat{x}\frac{\hat{d}}{dx}\right)$

$[\hat{A},\hat{B}]f = (\hat{A}\hat{B} - \hat{B}\hat{A})f = x\frac{d}{dx}f - \left(1 + x\frac{d}{dx}\right)f = -1\cdot f \quad \rightarrow \left[\frac{d}{dx}, x\right] = 1$

$\left[x, \frac{d}{dx}\right]$ $\quad \hat{x}\frac{\hat{d}}{dx} - \frac{\hat{d}}{dx}\hat{x}$

$\left(x + \frac{d}{dx}\right)^2 \rightarrow \left(x + \frac{d}{dx}\right)^2 f = \left(\hat{x}^2 + \frac{\hat{d}}{dx}\hat{x} + \hat{x}\frac{\hat{d}}{dx} + \frac{\hat{d}^2}{dx^2}\right)f$

$= x^2 f + \frac{d}{dx}xf + xf' + f'' = x^2 f + f + 2xf' + f'' = \left(x^2 + 1 + 2x\frac{d}{dx} + \frac{d^2}{dx^2}\right)f$

$x\frac{d}{dx} - \frac{d}{dx}x = -1 \Rightarrow \frac{d}{dx}x = x\frac{d}{dx} + 1$ $\Updownarrow$ stejné

$\left(\hat{x}^2 + \underline{\underline{\frac{\hat{d}}{dx}\hat{x}}} + \hat{x}\frac{\hat{d}}{dx} + \frac{d^2}{dx^2}\right) = \left(x^2 + x\frac{d}{dx} + 1 + x\frac{d}{dx} + \frac{d^2}{dx^2}\right) = \left(\hat{x}^2 + \hat{1} + 2\hat{x}\frac{\hat{d}}{dx} + \frac{\hat{d}^2}{dx^2}\right)$

[,]

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$$\frac{d^2}{dx^2} x^2 f = \frac{d}{dx}\left(2x f + x^2 f'\right) = 2f + 2xf' + 2xf' + x^2 f''$$

$$= \left(2 + 4x\frac{d}{dx} + x^2\frac{d^2}{dx^2}\right) f$$

$$\frac{d^2}{dx^2} x^2 = \frac{d}{dx}\underbrace{\left(\frac{d}{dx}x\right)}_{\hookrightarrow\, x\frac{d}{dx}+1}x = \frac{d}{dx}\left[x\frac{d}{dx}+1\right]x = \frac{d}{dx}x\frac{d}{dx}x + \frac{d}{dx}x =$$

$$= \left[x\frac{d}{dx}+1\right]\left[x\frac{d}{dx}+1\right] + x\frac{d}{dx} + 1 = x\underbrace{\frac{d}{dx}x}_{x\frac{d}{dx}+1}\frac{d}{dx} + 2x\frac{d}{dx} + x\frac{d}{dx} + 2$$

$$= x\left[x\frac{d}{dx}+1\right]\frac{d}{dx} + 3x\frac{d}{dx} + 2 = x^2\frac{d^2}{dx^2} + 4x\frac{d}{dx} + 2 \leftarrow$$

$$\frac{d}{dx}x^2 = \left(\frac{d}{dx}x\right)x = \left[x\frac{d}{dx}+1\right]x = x\frac{d}{dx}x + x = x\left[x\frac{d}{dx}+1\right] + x$$

$$= x^2\frac{d}{dx} + 2x$$

OK

$$\frac{\hat{d}}{dx}\hat{x}^2 f(x) = 2x f(x) + x^2 f' = \left[2x + x^2\frac{d}{dx}\right] f$$

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mějme $\hat{A}, \hat{B}$; $[\hat{A}, \hat{B}] = 1$ $\quad AB - BA = 1$

$$[A, B^2] = ? = AB^2 - B^2A = ABB - BAB + BAB - BBA$$

$$= \underbrace{[A,B]}_{1}B + B\underbrace{[A,B]}_{1} = 2B$$

~~AB~~

Mějme $\hat{A}, \hat{B}, \hat{C}$

čemu je rovno $[\hat{A} + \hat{B}, \hat{C}]$

expl. ověřit pro $\hat{A} = x$, $B = \frac{d}{dx}$, $C = x^2$, $f(x) = x$

$$\left[x + \frac{d}{dx}, x^2\right]x = \left(x + \frac{d}{dx}\right)x^2 \cdot x - x^2\left(x + \frac{d}{dx}\right)x$$

$$= x^4 + 3x^2 - x^4 - x^2 = 2x^2$$

$$\left[x + \frac{d}{dx}, x^2\right] = [x, x^2] + \left[\frac{d}{dx}, x^2\right] = \frac{d}{dx}x^2 - x^2\frac{d}{dx} = \frac{d}{dx}x^2 - x\frac{d}{dx}x + x\frac{d}{dx}x - x^2\frac{d}{dx}$$

$$= \left[\frac{d}{dx}, x\right]x + x\left[\frac{d}{dx}, x\right] = 2x$$

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· fce $\frac{1}{\sqrt{\pi}}\sin\phi$, $\cos\phi$ $\quad \phi\in(0,2\pi)$

$\sin 2\phi$, $\cos 2\phi$

$$\frac{1}{\pi}\int_0^{2\pi}\sin^2\phi\, d\phi = \frac{1}{\pi}\cdot\cancel{\pi}\left(\frac{1}{2}\;2\pi\right) = 1 \quad \text{OK}$$

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fce $\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$, $\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$, $\frac{1}{\sqrt{2\pi}}$

$$\hat{A} = \frac{d}{d\phi} \qquad \hat{B} = e^{i\phi}$$

$$\hat{A}\hat{B} = \frac{d}{d\phi}e^{i\phi}f(\phi) = ie^{i\phi}f(\phi) + e^{i\phi}f'(\phi) = \left(ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}\right)f$$

$$\hat{B}\hat{A} = e^{i\phi}\frac{d}{d\phi}f(\phi) \quad \text{dane}$$

$$[\hat{A},\hat{B}]f = \left(ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}\right)f - e^{i\phi}\frac{d}{d\phi}f = ie^{i\phi}f$$

$$\hat{A}\hat{B} - \hat{B}\hat{A} = ie^{i\phi}$$

$$\frac{d}{d\phi}e^{i\phi} = ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}$$

$$A^2B^2f = \frac{d^2}{d\phi^2}e^{i\phi}f(\phi) = \frac{d}{d\phi}\left(ie^{i\phi}f + e^{i\phi}f'\right) = -e^{i\phi}f + ie^{i\phi}f'$$

$$+ie^{i\phi}f' + e^{i\phi}f'' = \left[-e^{i\phi} + 2ie^{i\phi}\frac{d}{d\phi} + e^{i\phi}\frac{d^2}{d\phi^2}\right]f$$

$$\frac{d}{d\phi}\frac{d}{d\phi}e^{i\phi} = \frac{d}{d\phi}\left[ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}\right] = i\left[ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}\right] + \left[ie^{i\phi} + e^{i\phi}\frac{d}{d\phi}\right]\frac{d}{d\phi}$$

$$= -e^{i\phi} + 2ie^{i\phi}\frac{d}{d\phi} + e^{i\phi}\frac{d^2}{d\phi^2}$$

· Nora, 06