- relevance QM
- LA & QM

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relevance - de Broglie relation

Einstein: $E = \hbar\omega = \frac{h}{2\pi} 2\pi\nu = h\nu$ — photon energy depends on its frequency (colour)

photon: also $p = \hbar k = \frac{h}{\lambda}$ from Planck's law bb radiation

$E = pc$ (relativity with $m=0$)

$\lambda\nu = c$ (# oscillations × length of 1 oscillation)

$\hbar\omega = pc$

$\hbar\omega = p\lambda\nu$

$\frac{h}{2\pi} 2\pi \cancel{\nu} = p\lambda\cancel{\nu} \Rightarrow p = \frac{h}{\lambda}$

de Broglie: $p = \frac{h}{\lambda}$ holds in general

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

$\lambda = \frac{h}{p} \leftarrow 6{,}626 \cdot 10^{-34}\ m^2\,kg/s$; $\lambda = \frac{h}{\sqrt{2mE}}$

1) me (80kg) crashing from bicycle at 10 m/s

$p = mv = 800\ \frac{kg\,m}{s}$

$\lambda = \frac{6{,}626 \cdot 10^{-34}}{800} = 8{,}25 \cdot 10^{-37}\ m$

2) C_{60} molecule → mass $= 60 \cdot 12{,}01 \cdot 1{,}66 \cdot 10^{-27}\ kg \doteq 1{,}2 \cdot 10^{-24}\ kg$

60 — carbon — atomic mass unit

$v = 200\ m/s$

$\Rightarrow p = 2{,}4 \cdot 10^{-22}\ kg\,m/s$

$\lambda = \frac{6{,}626 \cdot 10^{-34}}{2{,}4 \cdot 10^{-22}} \doteq 2{,}76 \cdot 10^{-12}\ m$ (= pm) Arndt et al Nature 401 680 (1999)

3) electron ~~with~~ ~~from~~ ~~eV~~ 1eV

$\Rightarrow$ atomic units : $E = [Ha]$, $[m] = m_e$, $\hbar = 1 = \frac{e^2}{4\pi\varepsilon_0}$

~~E~~ $1eV \doteq \frac{1}{27.2}\ Ha$

$\lambda = \frac{2\pi\hbar^{\to 1}}{\sqrt{2mE}_{\to 1}} \overset{a.u.}{=} \frac{2\pi}{\sqrt{2E}} = \frac{2\pi}{\sqrt{\frac{1}{13.6}}} = \frac{2\pi}{\sqrt{\frac{1}{13.6}}} = 2\pi \cdot 3.7 = 23.2\ b$

what? Bohr

1 Bohr = 0.529 Å

what?

what? Ångström

$1Å = 10^{-10}\ m$

OK :)

$23.2b \doteq 12.3Å = 1.23 \cdot 10^{-9}\ m$

4) free particle with temperature T

$E = \frac{3}{2} k_B T$; $k_B = 1,3806 \cdot 10^{-23} J K^{-1}$

$\rightarrow$ to a.u.

$1 eV = 1,602 \cdot 10^{-19} J$
$1 eV = \frac{1}{27,2}$ Ha

$\Big\} \rightarrow 1.602 \cdot 10^{-19} J = \frac{1}{27.2}$ Ha

$43,57 \cdot 10^{-19} J =$ Ha

$J = 2,295 \cdot 10^{17}$ Ha

$k_B = 1,3806 \cdot 10^{-23} J K^{-1}$
$= 1,3806 \cdot 10^{-23} \cdot 2,295 \cdot 10^{17}$ Ha K^{-1}
$= 3,1685 \cdot 10^{-6}$ Ha K^{-1}

$\rightarrow E = \frac{3}{2} \cdot 3,1685 \cdot 10^{-6} \cancel{\text{Ha}K^{-1}} \cdot T$ [H ionisation $\approx \frac{1}{2}$ Ha $\Rightarrow 10^5$K]
(in reality $\sim 10^4$K only...)

$= 4,75275 \cdot 10^{-6} \cdot T$

$p = \sqrt{2mE} = \sqrt{2 \cdot 4,75275 \cdot 10^{-6}\, m\, T} = 3,083 \cdot 10^{-3} \sqrt{mT}$

EE) neutron ~~proton~~ $T = 110$ mK ; $m_n = 1839\, m_e$

$p = 3.083 \cdot 10^{-3} \sqrt{mT} = 3.083 \cdot 10^{-3} \sqrt{1839 \cdot 0,11} = 0.0438$

$\lambda = \frac{2\pi \overset{=1}{\hbar}}{p} = \frac{2\pi}{0.0438} = 143.3$ a.u.

1) ~~$\lambda = 2$Å, what is temperature~~

1) proton 20K:

$\lambda = \frac{2\pi\hbar}{\sqrt{2 m_p E}} = \frac{2\pi \overset{\to 1}{\hbar}}{\sqrt{2 \underbrace{m_p}_{1836 m_e} \frac{3}{2} k_B T}} = \frac{2\pi}{3,083 \cdot 10^{-3} \sqrt{m_p T}} = \frac{2\pi}{3,083 \cdot 10^{-3} \sqrt{1836 \cdot 20}}$

$= 10,66 \doteq 5,62$Å

2) proton 300K:

$\lambda = \frac{2\pi\hbar}{\sqrt{2 m_p E}} = \frac{2\pi}{3,083 \cdot 10^{-3} \sqrt{1836 \cdot 300}} = 2,746 = 1,45$Å

$\sim$ size of H-bond D

3) deuteron 300K

$\lambda = \lambda_{proton} \cdot \frac{1}{\sqrt{2}} \approx 1$Å $\longrightarrow$ don't drink heavy water too much!

Operátory 2022-ukol T13

$\frac{d}{dx}(f+g) = f' + g'$

$\frac{d}{dx}(cf) = c\frac{df}{dx}$

$\hat{O} = \frac{1}{f}$: $O(f+g) = \frac{1}{f+g}$

$O(f) = \frac{1}{f}$ $O(g) = \frac{1}{g}$

$O(f) + O(g) \neq O(f+g)$

$\frac{1}{\sqrt{\pi}}\sin(n\phi), \frac{1}{\sqrt{\pi}}\cos(n\phi), \frac{1}{\sqrt{2\pi}}$; $(0, 2\pi)$, $n \in \mathbb{N}$

normalizace: $f = \frac{1}{\sqrt{\pi}}\sin(n\phi)$

$$\int_0^{2\pi} f^* f \, d\phi = \frac{1}{\pi}\int_0^{2\pi} \sin^*(n\phi)\sin(n\phi)\, d\phi$$

$$= \frac{1}{\pi}\int_0^{2\pi}\frac{1}{(2i)^2}\left[e^{in\phi} - e^{-in\phi}\right]^2 d\phi$$

$$= \frac{1}{\pi}\int_0^{2\pi}\left(-\frac{1}{4}\right)\left[e^{2in\phi} + e^{-2in\phi} - 2\right] d\phi$$

$$= \frac{1}{\pi}\int_0^{2\pi}\frac{1}{2}\, d\phi = \frac{1}{2\pi}\cdot 2\pi = \underline{\underline{1}} \quad \text{OK}$$

$f = \frac{1}{\sqrt{\pi}}\sin(n\phi)$

$g = \frac{1}{\sqrt{\pi}}\cos(n\phi)$

$$\int_0^{2\pi} f^* g \, d\phi = \frac{1}{\pi}\int_0^{2\pi}\sin(n\phi)\cos(n\phi)\, d\phi$$

$$= \frac{1}{\pi}\frac{1}{4i}\int_0^{2\pi}\left[e^{in\phi} - e^{-in\phi}\right]\left[e^{in\phi} + e^{-in\phi}\right] d\phi$$

$$= \frac{1}{4\pi i}\int_0^{2\pi} e^{2in\phi} - e^{-2in\phi}\, d\phi = \underline{\underline{0}} \quad \text{OK}$$

$\hat{A} = i\frac{d}{d\phi}$

$\hat{A}\frac{1}{\sqrt{\pi}}\sin\phi = \frac{1}{\sqrt{\pi}}\cos\phi$ $\quad \hat{A}\frac{1}{\sqrt{\pi}}\sin\phi = -\frac{1}{\sqrt{\pi}}\cos\phi$ $\quad \hat{A}\frac{1}{\sqrt{2\pi}} = 0$

$\hat{B} = \sin\phi$

$\hat{B}\frac{1}{\sqrt{\pi}}\sin\phi = \frac{1}{\sqrt{\pi}}\sin^2\phi = \frac{1}{\sqrt{\pi}}\left[\frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right)\right]^2 = \frac{1}{\sqrt{\pi}}\frac{1}{-4}\left[e^{2i\phi} + e^{-2i\phi} - 2\right]$

$= \frac{1}{\sqrt{\pi}}\left[\frac{1}{2} - \frac{1}{2}\cos(2\phi)\right]$ ← kombinace 2 fcí, to je OK (není to vlastní stav)

$\hat{B}\frac{1}{\sqrt{\pi}}\cos\phi = \frac{1}{\sqrt{\pi}}\cos\phi\sin\phi = \frac{1}{\sqrt{\pi}}\frac{1}{4i}\left(e^{i\phi} + e^{-i\phi}\right)\left(e^{i\phi} - e^{-i\phi}\right) = \frac{1}{4i\sqrt{\pi}}\left(e^{2i\phi} - e^{-2i\phi} + 0\right)$

$= \cancel{\frac{1}{4i\sqrt{\pi}}}\ \frac{1}{2\sqrt{\pi}}\sin(2\phi)$

$\hat{B}\frac{1}{\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}}\sin\phi$