$E = \hbar\omega$ $\omega = 2\pi\nu$ $E = \hbar\, 2\pi\nu = h\nu$

$p = \hbar k$ $k = \frac{2\pi}{\lambda}$ $k\lambda = 2\pi$ $e^{i(kx \mp \omega t)}$

so that we have some useful quantity...?

photon $\lambda\nu = c$ (nebo ν)

ν - oscillations per sec

length of one oscillation

ν - times per sec

length per sec.

$$p = \hbar\frac{2\pi}{\lambda} = \hbar\frac{2\pi\nu}{c} = \frac{\hbar\omega}{c} \rightarrow \lambda = \frac{h}{p}$$

electron

$$\frac{\hbar^2\omega^2}{2m_0c^2} = \hbar\omega$$

$\hbar\omega = 2m_0c^2$

$\frac{\hbar\omega}{2} = m_0c^2$

$$\oint p\,dq = nh$$

$$p\psi(x) = -i\hbar\frac{d}{dx}\psi(x)$$

$$= -i\hbar\frac{\partial}{\partial x}e^{i(kx-\omega t)} = -i\hbar\, ik = \hbar k$$

21.1. Úvodní příklady

$\boxed{0}$

de Broglie vln. délka

$$\lambda = \frac{h}{p} \qquad \hbar = \frac{h}{2\pi}$$

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

částic s energií E_0, $E_0 = \frac{p^2}{2m}$ $p = \sqrt{2mE}$

v a.u.: elektron s $1eV = \frac{1}{27.2}$ Ha

$$\frac{p^2}{2\underset{1}{m}} = \frac{1}{27.2}$$

$$p^2 = \frac{1}{13.6}$$

$$\lambda = \frac{2\pi\overset{1}{\hbar}}{\sqrt{\frac{1}{13.6}}} = 2\pi\sqrt{13.6} = 2\pi\cdot 3.688$$

$= 23.2\ b$

$= 12.3\,Å = 1.23\cdot 10^{-9}\,m$

pro 1 b rozlišení ($=\lambda$)

$$\lambda = \frac{2\pi\hbar}{\sqrt{2mE}} \rightarrow 1 = \frac{2\pi}{\sqrt{2E}}$$

$$E = 2\pi^2 = 19.7\,Ha = 537\,eV, \text{ ok}$$

p+ s energií 1eV

$$\lambda = \frac{2\pi\hbar}{\sqrt{2m_pE}} \qquad m_p = 1836\,m_e$$

$$\lambda = \frac{2\pi\hbar}{\sqrt{2\cdot 1836\,m_e\,\frac{1}{27.2}}} = \frac{2\pi}{\sqrt{135}} = \frac{2\pi}{11.62} = 0.541\,b = 0.286\,Å$$

$= 2.86\cdot 10^{-11}\,m$

$m_e = 9.109 \cdot 10^{-31}\ kg$

$e = 1.602 \cdot 10^{-19}\ C$

$\hbar = 1.055 \cdot 10^{-34}\ J.s$

$\frac{1}{4\pi\varepsilon_0} = 8.988 \cdot 10^{9}\ kg\, m^3\, s^{-2}\, C^{-2}$

$1\,Ha = 4.360 \cdot 10^{-18}\ J$

time a.u $= 2.419 \cdot 10^{-17}\ s$

$k_B = 1.3806 \cdot 10^{-23}\ J K^{-1}$

---

zápisemka à 40% → 80% — MS do 7. týdne a do 14. týdne včetně

10% aktivita na cvičeních

10% domácí úkoly

10. 3. off

molekula UF_6 $=(238.06 + 6 \cdot 18.998)\, m_u = 352.048\, m_u$ UKM-T1.2

$m_u \doteq 1822.9\, m_e$ $\doteq 641748.3\, m_e$

$$\lambda = \frac{2\pi\hbar}{\sqrt{2mE}} = \frac{2\pi}{\sqrt{2\cdot 641748.3 \cdot \frac{1}{27.2}}} = \frac{2\pi}{\sqrt{47187.37}} = \frac{2\pi}{217.23} = 0.0289a_0$$

$$= 0.0153\,\text{Å} = 1.53\cdot 10^{-12}\,m$$

volná částice $E = \frac{3}{2} k_B T$ @300K: $\frac{3}{2} \cdot 1.3806 \cdot 10^{-23} \cdot T =$

$k_B = 1.3806 \cdot 10^{-23}\, JK^{-1}$

$$p = \sqrt{2m \frac{3}{2} k_B T} = \sqrt{3 m k_B T}$$

$k_B = 1.3806 \cdot 10^{-23}\, JK^{-1}$

$1eV = 1.602 \cdot 10^{-19}\, J$

$1eV = \frac{1}{27.2}\, Ha$

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

$43.57 \cdot 10^{-19}\, J = Ha$

$0.4357 \cdot 10^{-17}\, J = Ha$

$0.4357\, J = 10^{17}\, Ha$

$J = 2.295 \cdot 10^{17}\, Ha$

$k_B = 1.3806 \cdot 10^{-23} \cdot 2.295 \cdot 10^{17}\, Ha\, K^{-1}$

$= 3.1685 \cdot 10^{-6}\, Ha\, K^{-1}$

$$p = \sqrt{3 m k_B T} = \sqrt{3 \cdot 3.1685 \cdot 10^{-6}\, m T} = 3.083 \cdot 10^{-3} \sqrt{mT}$$

proton at 20K:

$$\lambda = \frac{2\pi\hbar}{\sqrt{2m_p E}} = \frac{2\pi\hbar}{\sqrt{2 m_p \frac{3}{2} k_B T}} = \ldots = \frac{2\pi}{3.083\cdot 10^{-3}\sqrt{20 \cdot 1836}} = \frac{2\pi}{3.083\cdot 10^{-3}\sqrt{36720}}$$

$$= \frac{2\pi}{0.003083 \cdot 191.62} = \frac{2\pi}{0.5907} = 10.636 = 5.62\,\text{Å}$$

looks OK

proton with 1eV

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

$\frac{p^2}{2m} = \frac{3}{2} k_B T$

$1 = \frac{3}{2} \cdot 8.62 \cdot 10^{-5}\, eV\, K^{-1}\, T$

$1 = 0.0001293\, K^{-1}\, T$

$T = 7734\, K$

@300K

$$= \frac{2\pi}{3.083\cdot 10^{-3}\sqrt{300 \cdot 1836}}$$

$$= \frac{2\pi}{3.083\cdot 10^{-3} \cdot 742} = \frac{2\pi}{2.288}$$

$= 2.746\, b = 1.45\,\text{Å}$

~ about the size of atomic bond or H-bond 888

21. 1. 14

UKM – T1.3

diffrakce He^4 na krystalu s SC mřížkou a $d = 0.2\,nm$
odhadněte, při jaké teplotě bude difrakce pozorovatelná

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

de Broglie : $\lambda = \frac{2\pi\hbar}{p}$

$$E = \frac{p^2}{2m} \qquad p = \frac{2\pi\hbar}{\lambda}$$

$$E = \frac{4\pi^2\hbar^2}{2m\lambda^2} = \frac{2\pi^2\hbar^2}{m\lambda^2} = \frac{3}{2} k_B T$$

assume $\lambda \approx d$

$$\frac{2\pi^2\hbar^2}{md^2} = \frac{3}{2} k_B T$$

$$T = \frac{4\pi^2\hbar^2}{3k_B m d^2} = \frac{4\pi^2}{3 \cdot 3.1685 \cdot 10^{-6} \cdot 4 \cdot 1822.9 \cdot (3.78)^2}$$

$$= \frac{4\pi^2}{990303 \cdot 10^{-6}} = \frac{4\pi^2}{0.99} \doteq 39.9\,K$$

$m(He^4) \doteq 4 \cdot 1822.9\, m_e$

$k_B = 3.1685 \cdot 10^{-6}\, Ha\, K^{-1}$

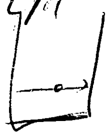
$d = 0.2\, nm = 2\,Å \doteq 3.78\, b$

$$\psi = e^{ikr} \qquad p = -i\hbar\frac{\partial}{\partial r}$$

$$p\psi = -i\hbar\frac{\partial}{\partial r} e^{ikr} = -i\hbar\, ik = \hbar k$$

Bohrův model

21.4/1



0 a

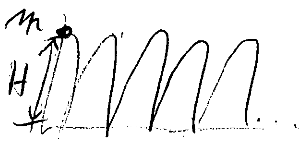
$$\oint p\,dx = \int_0^a p\,dx + \int_a^0 p\,dx = 2p\int_0^a dx = 2pa$$

$$= nh$$

$$p_n = \frac{nh}{2a}$$

$$E_n = \frac{p^2}{2m} = \frac{n^2h^2}{8ma^2} = \frac{n^2\hbar^2\pi^2}{2a^2m}$$

21.2/2



$$E = mgH \quad ; \quad E = \frac{p^2}{2m} + mgz$$

$$p = \pm\sqrt{(E-mgz)2m}$$

$$nh = \oint p\,dz = 2\int_0^H \sqrt{2m(E-mgz)}\,dz$$

$$= 2\sqrt{2m}\int_0^H \sqrt{E-mgz}\,dz \qquad E-mgz = t \qquad z=0 \to t=E$$

$$-mg\,dz = dt \qquad z=H \quad t=0$$

$$= 2\sqrt{2m}\int_E^0 t^{1/2}\left(-\frac{dt}{mg}\right) \cancel{dt}$$

$$= \frac{2\sqrt{2m}}{mg}\int_0^E t^{1/2}\,dt = \frac{2\sqrt{2m}}{mg}\,\frac{2}{3}\,t^{3/2}\Big|_0^E = \frac{2\sqrt{2m}}{mg}\,\frac{2}{3}\,E^{3/2}$$

$$nh = \frac{4\sqrt{2m}}{3mg}E^{3/2}$$

$$E^{3/2} = \frac{3mg\,nh}{4\sqrt{2m}} \;\rightarrow\; E_n = \left(\frac{3mg\,nh}{4\sqrt{2m}}\right)^{2/3} = \left(\frac{3m\sqrt{m}\,g\,nh}{4\sqrt{2}\,m}\right)^{2/3}$$

$$= \left(\frac{3m^{3/2}g\,nh}{4\sqrt{2}\,m}\right)^{2/3} = m\left(\frac{3g\,nh}{4\sqrt{2}\,m}\right)^{2/3} \quad \text{OK}$$

$$H_n = \frac{E}{mg} = \left(\frac{3nh}{4\sqrt{2}\,m}\right)^{2/3} g^{-1/3}$$

21.2/13 UKMTT-J

LHO s Bohrem

$$E = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \qquad \omega = \sqrt{\frac{k}{m}}$$

$$E_{tot} = \frac{m\omega^2 A^2}{2}$$ - integrál pohybu

$$\frac{p^2}{2m} = \frac{m\omega^2 A^2}{2} - \frac{m\omega^2 x^2}{2}$$

$$p^2 = m^2\omega^2 A^2 - m^2\omega^2 x^2 = m^2\omega^2 (A^2 - x^2)$$

$$p = m\omega\sqrt{(A^2 - x^2)}$$

$$nh = \oint p\, dx = 2\int_{-A}^{A} m\omega\sqrt{(A^2 - x^2)}\, dx = 2m\omega A \int_{-A}^{A} \sqrt{1 - x^2/A^2}\, dx =$$

integral from $\int_{A}^{-A}$

$x = -A \cos\varphi$

$dx = -A(-\sin\varphi)\, d\varphi$

$dx = A \sin\varphi\, d\varphi$

$= \cancel{2m\omega A}$

$-A = -A\cos(0)$

$A = -A\cos(\pi)$

$$= 2m\omega A \int_0^{\pi} \sqrt{1 - \cos^2\varphi}\; A\sin\varphi\, d\varphi$$

$$= 2m\omega A \int_0^{\pi} \sin^2\varphi\, A\, d\varphi = 2m\omega A^2 \underbrace{\int_0^{\pi} \sin^2\varphi\, d\varphi}_{=\pi/2}$$

$$= m\omega A^2 \pi$$

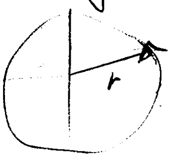
$$nh = m\omega A^2 \pi$$

$$A_n^2 = \frac{nh}{\pi m\omega} = \frac{2n\hbar}{m\omega}$$

$$E_n = \frac{m\omega^2}{2}\frac{2n\hbar}{m\omega} = n\hbar\omega$$ (quik correct $\frac{1}{2}\hbar\omega$ missing $\Delta x \Delta p$)

út 21.2/14

tuhý rotátor



$$L = T - \underset{0}{V} = \tfrac{1}{2} m v^2 = \tfrac{1}{2} m r^2 \dot\varphi^2$$

$$v = r\dot\varphi$$

$$p_\varphi = \frac{\partial L}{\partial \dot\varphi} = \tfrac{1}{2} m r^2 \frac{\partial \dot\varphi^2}{\partial \dot\varphi} = m r^2 \dot\varphi = \text{const}$$

$$nh = \cancel{\int_0^{2\pi} m r^2 \dot\varphi \, d\varphi = 2\pi} \int_0^{2\pi} p_\varphi \, d\varphi = 2\pi p_\varphi$$

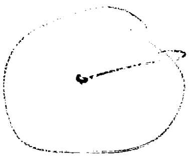
$$p_\varphi = n\hbar$$

$$H = \dot\varphi p_\varphi - L = m r^2 \dot\varphi^2 - \tfrac{1}{2} m r^2 \dot\varphi^2 = \tfrac{1}{2} m r^2 \dot\varphi^2$$

$$= \frac{p_\varphi}{m r^2} p_\varphi - L = \frac{p_\varphi^2}{2 m r^2} = \frac{1}{2}\frac{p_\varphi^2}{m r^2} = \frac{1}{2}\frac{p_\varphi^2}{I} = \frac{n^2\hbar^2}{2I}$$

(that's actually OK e⁻ in atoms...)

21.2/16 H-vodík



$$L = T - V = \tfrac{1}{2} m r^2 \dot\varphi^2 + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

- separace na úhlovou a radiální část:

úhel: $p_\varphi = \dfrac{\partial L}{\partial \dot\varphi} = m r^2 \dot\varphi$

$$\int_0^{2\pi} p_\varphi \, d\varphi = \int_0^{2\pi} \underbrace{m r^2 \dot\varphi}_{\text{const.}} \, d\varphi = m r^2 \dot\varphi \, 2\pi = nh$$

$$\dot\varphi_n = \frac{n\hbar}{m r^2} \quad \text{OK}$$

Coulomb síla = odstředivá

$$\frac{m_e v^2}{r} = \frac{m_e r^2 \dot\varphi^2}{r} = m_e r \dot\varphi^2 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$$

$$\dot\varphi_n = \frac{n\hbar}{m r^2} \quad \rightarrow \quad m r \frac{n^2\hbar^2}{m^2 r^4} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$$

$$\frac{n^2\hbar^2}{m} = \frac{1}{4\pi\varepsilon_0} e^2 r$$

$$r = \frac{n^2\hbar^2}{m}\frac{4\pi\varepsilon_0}{e^2}$$

for $n=1$ $= 1\,\text{a.u.}$ (1 Bohr) $= 0.529$ Å

21.2/6 cont'd

OKMT1-10

$$E = T + V = \frac{1}{2} m r^2 \dot\varphi_n^{\,2} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_n}$$

$\cancel{r = \ldots}$

$$= \cancel{\frac{1}{2} m r^2 \frac{n^2\hbar^2}{m^2 r^4} + \frac{e^2}{4\pi\varepsilon_0} \, m e^2}$$

$$\dot\varphi_n = \frac{n\hbar}{m r^2} = \frac{n\hbar}{m}\left(\frac{m e^2}{4\pi\varepsilon_0 \, n^2\hbar^2}\right)^2 \qquad r_n = \frac{n^2\hbar^2}{m}\,\frac{4\pi\varepsilon_0}{e^2}$$

$$= \frac{1}{2} m r^2 \cancel{\varphi} \frac{n^2\hbar^2}{m^2 r^4} - \frac{e^2}{4\pi\varepsilon_0}\,\frac{m e^2}{n^2\hbar^2 4\pi\varepsilon_0}$$

$$= \frac{1}{2}\frac{n^2\hbar^2}{m r^2} - \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{n^2\hbar^2} =$$

$$= \frac{1}{2}\frac{n^2\hbar^2}{m}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m^2}{n^4\hbar^4} - \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{n^2\hbar^2} =$$

$$= -\frac{1}{2}\frac{m}{n^2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \xrightarrow{\text{a.u.}} -\frac{1}{2n^2}\,[Ha]$$

(OK)

$E = \hbar\omega$

$\omega = 2\pi\nu$

$\nu = \frac{c}{\lambda}$

$E = \hbar\nu\, 2\pi = 2\pi\hbar\frac{c}{\lambda}$

c in a.u. $= 137$

$\frac{1}{2} = 2\pi\frac{137}{\lambda}$

$\lambda = 4\pi \cdot 137\; b = 1722\,b$

$= 91\,nm$

$\frac{1}{n^2}$ $\quad \frac{1}{4} - \frac{1}{9} = \frac{5}{36}$

$91\,nm \cdot \frac{36}{5} = 655\,nm$

(correct:)