Structure of matter: Homework to exercise 11

Harmonic oscillator/oscillator strength/H-atom

400 ~ 700 nm

Due on January 9th 2024 at noon

Please indicate your name on the solution sheets and send it to your seminar leader!

$n \Rightarrow \infty \quad \lambda = \frac{1}{\nu_{nm}} = \frac{9}{R_\infty} = \frac{9}{1.097\times10^5\ \mathrm{cm}} \cong 8\times10^{-4}\ \mathrm{cm} \cong 1.\ \mu m$

$\lambda = \frac{1}{R_\infty\left(\frac{1}{9}-\frac{1}{16}\right)} = \frac{1}{5.3\times10^3}\ \mathrm{cm} = 1.88\times10^{-4}\ \mathrm{cm} \approx 1.88\ \mu m$

1. Multiple-choice test: Please tick all box(es) with correct answer(s)!
   (correctly ticked box: +1/2 point; wrongly ticked box: -1/2 point)

The emission lines of the Paschen spectral series in a H-atom are observed in the Paschen $\nu_{nm} = R_\infty\left(\frac{1}{9}-\frac{1}{n^2}\right)$ $n>3$ $R_\infty = 1.097\times10^5\ \mathrm{cm}$	Infrared	✓
	visible	
	ultraviolet	
	γ-range	
In a H-atom, Bohrs radius is approximately equal to Bohr's radius $a_0 = \frac{\varepsilon_0 h^2}{e^2 \pi \mu} \approx 0.53\times10^{-10}\ \mathrm{m}$	0.05nm	✓
	$5*10^{-11}$m	✓
	10nm	

2. True or wrong? Make your decision (tick the appropriate box):

   (2 points): 1 point per correct decision, 0 points per wrong or no decision

$T_{kin} = -\frac{V(r)}{2} = \frac{1}{8\pi\varepsilon_0}\frac{Ze^2}{r}$

Assertion	true	wrong
In any circular Bohr orbit, the electrons kinetic energy is equal to its potential one.		✓
From the hydrogen emission spectrum, only certain lines of the Balmer series fall into the visible spectral range	✓	

$h\uparrow \Rightarrow \nu_{nm}\uparrow \Rightarrow \lambda\downarrow \quad \nu_{nm} = R_\infty\left(\frac{1}{4}-\frac{1}{n^2}\right) \quad n=3 \Rightarrow \lambda_{max} = \frac{1}{\nu_{nm}} = \frac{1}{R_\infty\left(\frac{1}{4}-\frac{1}{9}\right)} = 6.56\times10^{-7}\ \mathrm{m} = 656\ \mathrm{nm}$

$n \to \infty \quad \lambda_{min} = \frac{4}{R_\infty} = 3.64\times10^{-7}\ \mathrm{m} = 364\ \mathrm{nm}$

3. Calculate the expectation value of the potential energy in the eigenstate n=7 of a one-dimensional harmonic oscillator with resonance frequency ω_o! (4 Points)

4. What is the oscillator strength f_{nm} of a dipole-transition between the states

   - m=1 and n=51 in a 1D harmonic oscillator?
   - m=50 and n=51 in a 1D harmonic oscillator?
   - m=1 and n=3 for a quantum particle in a 1D box potential with infinitely high walls? (3 points)

5. Estimate the difference between the emission wavelength of the transition n =2 → n =1 in an ordinary hydrogen atom and a deuterium atom. (6 points)

   H^2

6. The following integral will become important for calculating relevant expectation values for the hydrogen atom. So please solve the integral:

$$\int_0^{\infty} x^n e^{-px} dx = ??$$ (n – integer; p>0) (6 points)

(3) $U = T_{kin} = \frac{1}{2}E_n = \frac{1}{2}\hbar\omega_0(n+\frac{1}{2})$

$n=7 \Rightarrow U = \frac{15}{4}\hbar\omega_0$

(4) ① $f_{nm} = \frac{2M_0}{\hbar}\omega_{nm}|X_{nm}|^2$ $\quad \omega_{nm} = \frac{E_n - E_m}{\hbar}$ $\quad E_n = \hbar\omega_0(n+\frac{1}{2}) \Rightarrow \omega_{51,1} = \frac{E_{51}-E_1}{\hbar} = 50\omega_0$

$X_{nm} = \langle n|x|m\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{m+1}\,\delta_{n,m+1} + \sqrt{m}\,\delta_{n,m-1})$ $\qquad \delta_{nm} = \begin{cases} 1 & n=m \\ 0 & n\neq 0 \end{cases}$

$\Rightarrow X_{nm} = \langle 51|x|1\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{2}\,\delta_{51,2} + \delta_{51,0}) = 0$

$\Rightarrow f_{51,1} = 0$

② $\sum_\ell f_{\ell n} = \frac{2m}{\hbar}\sum_\ell \omega_{\ell n}|X_{n\ell}|^2 = 1 \Rightarrow f_{n+1,n} + f_{n-1,n} = 1$

$n=0 \quad f_{1,0} + f_{-1,0} = f_{1,0} = 1$ $\qquad n=1 \quad f_{2,1} + f_{0,1} = f_{2,1} - f_{1,0} = 1 \Rightarrow f_{2,1} = 2.$

$n=2. \quad f_{3,2} + f_{1,2} = f_{3,2} - f_{2,1} = 1 \Rightarrow f_{3,2} = 3.$

$n=3. \quad f_{4,3} + f_{2,3} = f_{4,3} - f_{3,2} = 1 \Rightarrow f_{4,3} = 4$

$\Rightarrow f_{nm} = f_{51,50} = 51$

③ $\varphi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x \Rightarrow \varphi_{n=1} = \sqrt{\frac{2}{L}}\sin\frac{\pi}{L}x$ $\quad \varphi_{n=3} = \sqrt{\frac{2}{L}}\sin\frac{3\pi}{L}x$ $\quad E_n = \frac{h^2 n^2}{8mL^2}$ $\quad E_3 - E_1 = \frac{h^2}{mL^2}$

$\langle 3|x|1\rangle = \int_x \varphi_3^* x \varphi_1\, dx = \frac{2}{L}\int x\sin\frac{3\pi}{L}x\sin\frac{\pi}{L}x\, dx = \frac{1}{L}\int_0^L x(\cos\frac{2\pi}{L}x + \cos\frac{4\pi}{L}x)\, dx$

$= \frac{1}{L}\int_0^L x\cos\frac{2\pi}{L}x + \frac{1}{L}\int_0^L x\cos\frac{4\pi}{L}x\, dx = \frac{1}{2\pi}\int_0^L x\, d\sin\frac{2\pi}{L}x + \frac{1}{4\pi}\int_0^L x\, d\sin\frac{4\pi}{L}x$

$= \frac{1}{2\pi}\left(x\sin\frac{2\pi}{L}x\Big|_0^L - \int_0^L \sin\frac{2\pi}{L}x\,dx\right) + \frac{1}{4\pi}\left(x\sin\frac{4\pi}{L}x\Big|_0^L - \int_0^L \sin\frac{4\pi}{L}x\,dx\right)$

$= \frac{L}{4\pi^2}\cos\frac{2\pi}{L}x\Big|_0^L + \frac{L}{16\pi^2}\cos\frac{4\pi}{L}x\Big|_0^L = 0$

$\Rightarrow f_{nm} = \frac{2m}{\hbar}\omega_{nm}|X_{nm}|^2 = 0$

(5) Hydrogen atom: $R_y = \frac{e^4\mu}{8\varepsilon_0^2 h^2} \approx 13.6\,eV$ $\qquad E = -R_y\frac{Z^2}{n^2} = -R_y\frac{1}{n^2}$

$\omega_{nm} = \frac{E_n - E_m}{\hbar}$ $\quad \omega_{21} = \frac{E_2 - E_1}{\hbar} = -\frac{R_y}{\hbar}(\frac{1}{2^2} - 1) = \frac{3R_y}{4\hbar}$ $\quad \lambda_H = \frac{2\pi c}{\omega} = \frac{8\pi c\hbar}{3R_y}$ $\quad \lambda_D = \frac{8\pi c\hbar}{3R_y'}$

$\Delta\lambda = \frac{8\pi}{3}c\hbar\left(\frac{1}{R_y} - \frac{1}{R_y'}\right)$ $\quad R_y = \frac{e^4\mu}{8\varepsilon_0^2 h^2} = \frac{e^4}{8\varepsilon_0^2 h^2}\cdot\frac{m_p m_e}{m_p + m_e}$ $\quad R_y' = \frac{e^4}{8\varepsilon_0^2 h^2}\cdot\frac{2m_p m_e}{2m_p + m_e}$

$$\Rightarrow \Delta\lambda = \frac{8\pi}{3} c h \cdot \frac{8\varepsilon_0^2 h^2}{e^4}\left(\frac{2m_p+2m_e}{2m_p m_e} - \frac{2m_p+m_e}{2m_p m_e}\right) = \frac{32\varepsilon_0^2 h^3 c}{6 m_p e^4} = \frac{32\cdot(8.86)^2\cdot 10^{-24}\, F^2/m^2 \cdot 6.625^3\cdot 10^{-102}\, W^3 s^6 \cdot 3\times 10^8\, m/s}{6\cdot 1.672\times 10^{-27}\, kg \cdot 1.602^4\cdot 10^{-76}\, A^4 s^4}$$

$$= 3.316\times 10^{-11}\, m = 3.316\times 10^{-2}\, nm$$

$\int_0^{\infty} x^n e^{-px} dx = ??$ (n – integer; p>0) (6 points)

解

$$\int_0^{\infty} x^n e^{-px} dx = -\frac{1}{p}\int_0^{\infty} x^n de^{-px} = -\frac{1}{p}\left(x^n e^{-px}\Big|_0^{\infty} - \int e^{-px} dx^n\right) = \frac{1}{p}\int e^{-px} n x^{n-1} dx$$

$$= \frac{n}{p}\int_0^{\infty} e^{-px} x^{n-1} dx = -\frac{n}{p^2}\int x^{n-1} de^{-px} = -\frac{n}{p^2}\left(x^{n-1}e^{-px}\Big|_0^{\infty} - \int_0^{\infty} e^{-px} dx^{n-1}\right)$$

$$= \frac{n(n-1)}{p^2}\int_{-\infty}^{\infty} e^{-px} x^{n-2} dx$$

$$\cdots\cdots = \frac{n(n-1)\cdot(n-2)\cdots 2}{p^{n-1}}\int_0^{\infty} e^{-px} x\, dx = -\frac{n!}{p^n}\int_0^{\infty} x\, de^{-px} = -\frac{n!}{p^n}\left(x e^{-px}\Big|_0^{\infty} - \int e^{-px} dx\right)$$

$$= \frac{n!}{p^n}\int e^{-px} dx = -\frac{n!}{p^{n+1}} e^{-px}\Big|_0^{\infty} = \frac{n!}{p^{n+1}}$$