

# Structure of matter: Homework to exercise 11

## Harmonic oscillator/oscillator strength/H-atom

Due on **January 9<sup>th</sup> 2024 at noon**

$$400 \sim 700 \text{ nm}$$

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

$$n \rightarrow \infty \quad \lambda = \frac{1}{\text{nm}} = \frac{q}{R_\infty} = \frac{q}{(1.097 \times 10^5) \text{ cm}^{-1} \cdot 10^{-4} \text{ cm}} = \frac{1}{1.097 \times 10^{-9} \text{ m}} = \frac{1}{1.097 \times 10^{-9} \text{ m}} = 9.13 \times 10^8 \text{ m}^{-1}$$

$$\lambda = \frac{1}{R_\infty \left( \frac{1}{q} - \frac{1}{n} \right)} = \frac{1}{5.3 \times 10^{-3} \text{ cm}} = 1.88 \times 10^{-4} \text{ cm} = 1.88 \mu\text{m}$$

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	Infrared	<input checked="" type="checkbox"/>
	visible	<input checked="" type="checkbox"/>
	ultraviolet	<input checked="" type="checkbox"/>
	$\gamma$ -range	<input checked="" type="checkbox"/>
In a H-atom, Bohrs radius is approximately equal to Bohr's radius $a_0 = \frac{4\pi\hbar^2}{e^2\kappa\mu} \approx 0.53 \times 10^{-10} \text{ m}$	0.05nm	<input checked="" type="checkbox"/>
	$5 \times 10^{-11} \text{ m}$	<input checked="" type="checkbox"/>
	10nm	<input checked="" type="checkbox"/>

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

Assertion	$T_{kin} = \frac{1}{2} \frac{V(r)}{Ze^2}$	true	wrong
In any circular Bohr orbit, the electrons kinetic energy is equal to its potential one.		<input checked="" type="checkbox"/>	
From the hydrogen emission spectrum, only certain lines of the Balmer series fall into the visible spectral range,		<input checked="" type="checkbox"/>	

3. Calculate the expectation value of the potential energy in the eigenstate  $n=7$  of a one-dimensional harmonic oscillator with resonance frequency  $\omega_0$ ! (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  $n=2 \rightarrow n=1$  in an ordinary hydrogen atom and a deuterium atom. (6 points)



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

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

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

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



(4)  $f_{nm} = \frac{2m}{\pi} w_{nm} |x_{nm}|^2 \quad W_{nm} = \frac{E_n - E_m}{\pi} \quad E_n = \hbar \omega_0 (n + \frac{1}{2}) \Rightarrow W_{51,1} = \frac{E_{51} - E_1}{\pi} = 50 \hbar \omega_0$

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

$$\Rightarrow X_{nm} = \langle 5 | x | 1 \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{2} \delta_{5,2} + \delta_{5,0}) = 0$$

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

(5)  $\sum f_{en} = \frac{2m}{\pi} \sum (w_{en} |x_{en}|)^2 = 1 \Rightarrow f_{n+1,n} + f_{n-1,n} = 1$

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

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

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

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

(3)

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

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

$$= \frac{1}{L} \left[ x \cos \frac{2\pi}{L} x \Big|_0^L + \frac{1}{2} \int_0^L x \cos \frac{4\pi}{L} x dx \right] = \frac{1}{2\pi} \int_0^L x ds \sin \frac{2\pi}{L} x + \frac{1}{4\pi} \int_0^L x ds \sin \frac{4\pi}{L} x$$

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

$$= \frac{1}{4\pi^2} \cos \frac{2\pi}{L} x \Big|_0^L + \frac{1}{16\pi^2} \cos \frac{4\pi}{L} x \Big|_0^L = 0$$

$\Rightarrow f_{nm} = \frac{2m}{\pi} w_{nm} |x_{nm}|^2 = 0$

(5) Hydrogen atom :  $Ry = \frac{e^4 \mu}{8\pi^2 h^2} \approx 13.6 \text{ eV} \quad E = -Ry \frac{Z^2}{n^2} = -Ry \frac{1}{n^2}$

$$W_{nm} = \frac{E_n - E_m}{\pi} \quad W_{21} = \frac{E_2 - E_1}{\pi} = -\frac{Ry}{\pi} \left( \frac{1}{2^2} - 1 \right) = \frac{3Ry}{4\pi} \quad \lambda_{\mu} = \frac{2\pi c}{\nu} = \frac{8\pi c \hbar}{3Ry} \quad \lambda_{\mu} = \frac{8\pi c \hbar}{3Ry}$$

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

$$\Rightarrow \Delta \lambda = \frac{8\lambda}{3} \left( h \cdot \frac{8\epsilon_0^2 h^2}{Q^4} \left( \frac{2mp + 2me}{2mpme} - \frac{2mpme}{2mp + 2me} \right) \right) = \frac{32 \epsilon_0^2 h^3 C}{6mp e^4} = \frac{32 \cdot (8.86)^2 \cdot 10^{-24} \cdot F^2/m^2 \cdot 6.62 \cdot 10^{-34} \cdot W^3 S^6 \cdot 3 \times 10^8 m/s}{6 \cdot 1.672 \times 10^{-27} kg \cdot 1.602 \cdot 10^{-19} A^4 S^4}$$

$$= 3.36 \times 10^{-1} m = 3.36 \times 10^{-2} nm$$

(b)

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

$$\begin{aligned}
 b) \quad \int_0^\infty x^n e^{-px} dx &= -\frac{1}{p} \int_0^\infty x^n de^{-px} = -\frac{1}{p} (x^n e^{-px} \Big|_0^\infty - \int e^{-px} dx^n) = \frac{1}{p} \int e^{-px} n x^{n-1} dx \\
 &= \frac{n}{p} \int_0^\infty e^{-px} x^{n-1} dx = -\frac{n}{p^2} \int x^{n-1} de^{-px} = -\frac{n}{p^2} (x^{n-1} e^{-px} \Big|_0^\infty - \int_0^\infty e^{-px} dx^{n-1}) \\
 &= \frac{n(n-1)}{p^2} \int_0^\infty e^{-px} x^{n-2} dx \\
 &= \frac{n(n-1)(n-2)\dots2}{p^{n-1}} \int_0^\infty e^{-px} x dx = -\frac{n!}{p^n} \int_0^\infty x^n de^{-px} = -\frac{n!}{p^n} (x e^{-px} \Big|_0^\infty - \int e^{-px} dx) \\
 &= \frac{n!}{p^n} \int e^{-px} dx = -\frac{n!}{p^{n+1}} e^{-px} \Big|_0^\infty = \frac{n!}{p^{n+1}}
 \end{aligned}$$

(b)