

PHOT 222: Quantum Photonics

Final exam A: questions & solutions

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Exam Questions

Grading: The final exam counts for 60% of your total grade.

Exam type: Closed-book, all questions can be answered using only pen and paper. Calculators, mobile phones, laptops are not needed, and are not allowed to be used during the exam.

The duration of the exam is 3 hours.

This document contains both the problems and their solutions. Considering the score calculation:

- Each of the questions is valued equally in the total score.
- Subproblems (a , b , c , ...) within a question are weighed equally.
- Answers should contain: The final formula/expression together with its derivation and a numerical approximate value with the **correct units**.

Question 1: Compton scattering

An x-ray photon is scattered when hitting a free electron in a target during a Compton scattering experiment. The incident photon has wavelength λ_0 and energy $E_0 = 0.2$ MeV before scattering, and is scattered under an angle $\theta = 90^\circ$. The wavelength λ' of the photon after scattering is given by the Compton shift:

$$\lambda' - \lambda_0 = \lambda_C (1 - \cos(\theta)) \quad \text{with Compton wavelength } \lambda_C = \frac{h}{mc} \approx 2.4 \times 10^{-12} \text{ m}$$

- (a) What is the wavelength λ' of the photon after scattering?
- (b) How much energy is transferred to the electron? Would the electron be moving at a relativistic speed after the collision? (approximation to 1 significant figure is sufficient)

Solution (Q1)

(a) The wavelength of the photon after collision λ' can be obtained directly from the Compton shift formula $\lambda' = \lambda_0 + \lambda_C (1 - \cos(\theta))$, together with the fact that $\cos(90^\circ) = 0$:

$$\lambda' = \lambda_0 + \lambda_C = \frac{hc}{E_0} + \lambda_C = \frac{1240 \text{ eV nm}}{0.2 \times 10^6 \text{ eV}} + 2.4 \times 10^{-12} \text{ m} = 6.2 \times 10^{-3} \text{ nm} + 2.4 \times 10^{-3} \text{ nm}$$

Resulting in $\lambda' = 8.6 \times 10^{-3} \text{ nm}$ A relatively large increase in wavelength.

(b) To find the energy transferred to the electron, we subtract the energy of the photon after the collision from its initial energy E_0 :

$$\Delta E = E_0 - E' = E_0 - \frac{hc}{\lambda'} = 0.2 \text{ MeV} - \frac{1240 \text{ eV nm}}{8.6 \times 10^{-3} \text{ nm}} \approx 0.2 - 0.14 \text{ MeV},$$

which is approximately 0.06 MeV. This energy is more than 10% of the rest energy of an electron 0.511 MeV, and in case accurate results would be required it would be advised to use the relativistic description for the electron motion.

Question 2: Quantum Harmonic Oscillator

The time-independent Schrodinger equation for the harmonic oscillator is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x)$$

and the ground state is: $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$ with $E_0 = \frac{1}{2}\hbar\omega$

(a) Prove that the ground state wave function is indeed a solution of the time-independent Schrodinger equation with energy $E_0 = \frac{1}{2}\hbar\omega$ (write down sufficient in-between steps).

(b) Calculate the expectation value for the potential energy: $\frac{1}{2}m\omega^2\langle x^2 \rangle$ for the ground state ψ_0 .

Solution (Q2)

(a) To prove that the wave function $\psi_0(x)$ is a solution we first calculate its second derivative:

$$\begin{aligned} \frac{d^2\psi_0(x)}{dx^2} &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{d^2}{dx^2} \left(e^{-\frac{m\omega}{2\hbar} x^2}\right) \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{d}{dx} \left(-\frac{m\omega}{\hbar} x e^{-\frac{m\omega}{2\hbar} x^2}\right) \\ &= -\frac{m\omega}{\hbar} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(e^{-\frac{m\omega}{2\hbar} x^2} - \frac{m\omega}{\hbar} x^2 e^{-\frac{m\omega}{2\hbar} x^2}\right) \\ &= -\frac{m\omega}{\hbar} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2} \left(1 - \frac{m\omega}{\hbar} x^2\right) \\ &= -\frac{m\omega}{\hbar} \left(1 - \frac{m\omega}{\hbar} x^2\right) \psi_0 \end{aligned}$$

Then we fill it in in the left-hand-side of the time-independent Schrodinger equation:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi_0(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi_0(x) &= \frac{\hbar^2}{2m} \frac{m\omega}{\hbar} \left(1 - \frac{m\omega}{\hbar} x^2\right) \psi_0 + \frac{1}{2}m\omega^2 x^2 \psi_0(x) \\ &= \frac{\hbar\omega}{2} \psi_0(x) - \frac{1}{2}m\omega^2 x^2 \psi_0(x) + \frac{1}{2}m\omega^2 x^2 \psi_0(x) \\ &= \frac{\hbar\omega}{2} \psi_0(x) \end{aligned}$$

Therefore we end up with the correct term on the right-hand-side: $\frac{\hbar\omega}{2}\psi_0(x)$, proportional to the wave function, meaning that $\psi_0(x)$ is a solution of the time-independent Schrodinger equation and the corresponding eigenenergy is indeed $E_0 = \frac{\hbar\omega}{2}$.

(b) To calculate the expectation value for the potential energy: $\langle V(x) \rangle = \frac{1}{2}m\omega^2 \langle x^2 \rangle$, we first calculate $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 |\psi_0|^2 dx = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{+\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} dx = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \frac{\hbar}{2m\omega} \sqrt{\frac{\pi\hbar}{m\omega}} = \frac{\hbar}{2m\omega}$$

Now we multiply with the prefactor:

$$\langle V(x) \rangle = \frac{1}{2}m\omega^2 \langle x^2 \rangle = \frac{1}{2}m\omega^2 \frac{\hbar}{2m\omega} = \frac{1}{4}\hbar\omega$$

which tells us that the expectation value of the potential energy is half of the expectation value of the Hamiltonian (i.e. the energy).

Question 3: 3D Particle in a Box

Assume a quantum particle with rest energy $mc^2 = 6.2$ MeV in a 3D box of dimensions $L \equiv L_x = L_y = L_z = 0.5$ nm (a cubic box).

(a) Calculate the energy of the ground state (in eV).

(b) Assume that the system transitions from a state with quantum numbers $n_x = 3$, $n_y = 1$, $n_z = 1$, to the ground state, by emitting a photon. What is the frequency of the photon (approximately)?

Solution (Q3)

(a) The ground state has quantum numbers: $n_x = 1$, $n_y = 1$, $n_z = 1$, where the quantum numbers cannot be zero otherwise the wave function is not normalizable. The energy is then given by:

$$E_{1,1,1} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) = \frac{\hbar^2 c^2}{8mc^2 L^2} (1+1+1) = 3 \cdot \frac{(1240)^2 \text{ eV}^2 \text{ nm}^2}{8 \cdot 6.2 \text{ eV} \cdot 0.5^2 \text{ nm}^2} = 3 \cdot 0.124 \text{ eV}$$

(b) The state with $n_x = 3$, $n_y = 1$, $n_z = 1$ has an energy proportional to the ground state where only the factor $(n_x^2 + n_y^2 + n_z^2) = 11$ is different:

$$E_{3,1,1} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) = 11 \cdot 0.124 \text{ eV}$$

When transitioning to the ground state by emitting a photon the frequency f of the photon can be derived from the energy difference $hf = \Delta E = E_{3,1,1} - E_{1,1,1} \approx 1 \text{ eV}$:

$$f = \frac{1}{h} (E_{3,1,1} - E_{1,1,1}) = \frac{8 \cdot 0.124 \text{ eV}}{4.14 \times 10^{-15} \text{ eV s}} \approx 2.4 \times 10^2 \text{ THz}$$

which is in the infrared range as expected for an energy $hf \approx 1 \text{ eV}$.

Question 4: Quantum hydrogen atom model

A hydrogen atom has energy equal to $E_n = -1.511 \text{ eV}$.

- (a) What is the principal quantum number n ?
- (b) What are the possible orbitals for the electron to be in (ignore superposition states), write down all possible combinations of quantum numbers: n, l, m_l .

Solution (Q4)

- (a) The principal quantum number n can be found from:

$$E_n = -\frac{\text{Ry}}{n^2} \Rightarrow n^2 = -\frac{\text{Ry}}{E_n} = \frac{13.6 \text{ eV}}{1.511 \text{ eV}} \Rightarrow \frac{10}{2} < n^2 < \frac{15}{1.5} \Rightarrow 5 < n^2 < 10$$

Where we squeezed the actual value between easy-to-calculate numerical values. The only positive integer number n fulfilling the last condition is $n = 3$.

- (b) From above we know that $n = 3$ is a fixed value. For $n = 3$ the quantum number l can have values $l = 0, 1, 2$, corresponding to s, p, and d orbitals. For a specific value of l , the magnetic orbital quantum number can take values $m_l = -l, \dots, -1, 0, 1, \dots, l$, this gives us the following combinations:

3s orbital (1 orbital): $n = 3, l = 0$, and $m = 0$.

3p orbitals (3 orbitals): $n = 3, l = 1$, and $m = -1, 0, 1$.

3d orbitals (5 orbitals): $n = 3, l = 2$, and $m = -2, -1, 0, 1, 2$.

Alternatively, we can write them as down as explicit combinations (n, l, m_l) :

$$\begin{aligned} \text{3s orbital :} & \quad (3, 0, 0), \\ \text{3p orbitals :} & \quad (3, 1, -1), (3, 1, 0), (3, 1, 1), \\ \text{3d orbitals :} & \quad (3, 2, -2), (3, 2, -1), (3, 2, 0), (3, 2, 1), (3, 2, 2) \end{aligned}$$

Question 5: Effective atomic number/charge

A sodium atom (Na) in the ground state has configuration $1s^2 2s^2 2p^6 3s^1$. The spectrum in the figure shows some of the possible transitions of the valence electron with corresponding (excitation/emission) wavelengths in nm.

- (a) What is the energy of the 5s state (derive using given transition wavelengths and value of $E_{3s} = -5.12 \text{ eV}$)?
- (b) What is the effective atomic number Z_{eff} for the 3s state?

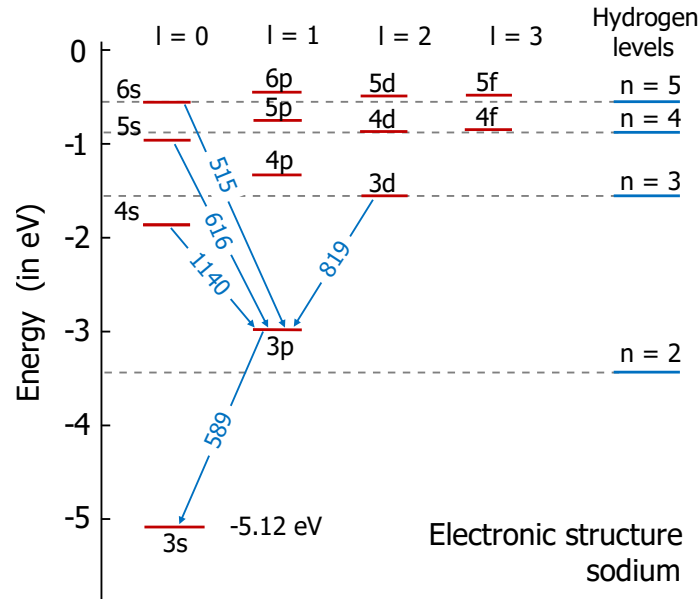


Figure 1: Energy spectrum of sodium for energy-levels from 3s (valence electron in the ground state) and above. The transition wavelengths for emission are shown for some of the allowed transitions (in nm)

Solution (Q5)

(a) To find the energy E_{5s} of the 5s state we calculate the energy differences between the E_{3p} and E_{3s} and between E_{5s} and E_{3p} :

$$\Delta E_1 = E_{3p} - E_{3s} = \frac{hc}{589 \text{ nm}} = \frac{1240 \text{ eV nm}}{589 \text{ nm}} \approx \frac{124}{59} \text{ eV} \approx \left(2 + \frac{6}{59}\right) \text{ eV} \approx 2.1 \text{ eV}$$

$$\Delta E_2 = E_{5s} - E_{3p} = \frac{hc}{616 \text{ nm}} = \frac{1240 \text{ eV nm}}{616 \text{ nm}} \approx 2 \text{ eV}$$

Resulting in an energy difference $\Delta E = E_{5s} - E_{3s} = \Delta E_1 + \Delta E_2 = 4.1 \text{ eV}$:

$$E_{5s} = E_{3s} + \Delta E \approx (-5.12 + 4.1) \text{ eV} \approx -0.98 \text{ eV}$$

Where the approximation is relatively rough, and $E_{5s} = -1.0 \text{ eV}$ is a more faithful presentation of the accuracy with correct significant figures.

(b) The effective atomic number Z_{eff} for the 3s state can be derived from:

$$E_{3s} = -\frac{Z_{\text{eff},3s}^2 \text{ Ry}}{3^2} \Rightarrow Z_{\text{eff},3s} = \sqrt{\frac{9 \cdot E_{3s}}{-\text{Ry}}} = \sqrt{\frac{-9 \cdot 5.12 \text{ eV}}{-13.6 \text{ eV}}} = \sqrt{\frac{9 \cdot 5.12}{13.6}}$$

For which we can find a (very rough) approximate value:

$$Z_{\text{eff},3s} \approx \sqrt{\frac{46}{13.6}} \approx \sqrt{3 + \frac{5.2}{13.6}} \approx \sqrt{3.4} \approx 1.8$$

Question 6: Free electron model

The Fermi-energy E_F corresponds to the highest occupied energy level at zero temperature and is related to the electron concentration n_e by $E_F \approx (0.36 \times 10^{-18} \text{ eV m}^2) \cdot n_e^{2/3}$.

(a) Calculate the Fermi-energy of sodium (Na) using the electron concentration n_e reported in the table below.

(b) Sketch the density of states $g(E)$, the Fermi-dirac distribution $f(E)$, and the electron density $N(E) = g(E) f(E)$ as function of the energy for a typical metal (i.e. free electron model). Indicate where the Fermi-energy is.

Metal	n_e (in 10^{28} m^{-3})	Fermi energy (eV)
Li	4.70	4.72
Na	≈ 2.70	?
K	1.40	2.12
Cu	8.46	7.05
Ag	5.85	5.48
Au	5.90	5.53

Figure 2: Table with theoretical values of the Fermi Energy for Metals at 300 K Based on the Free-Electron Theory

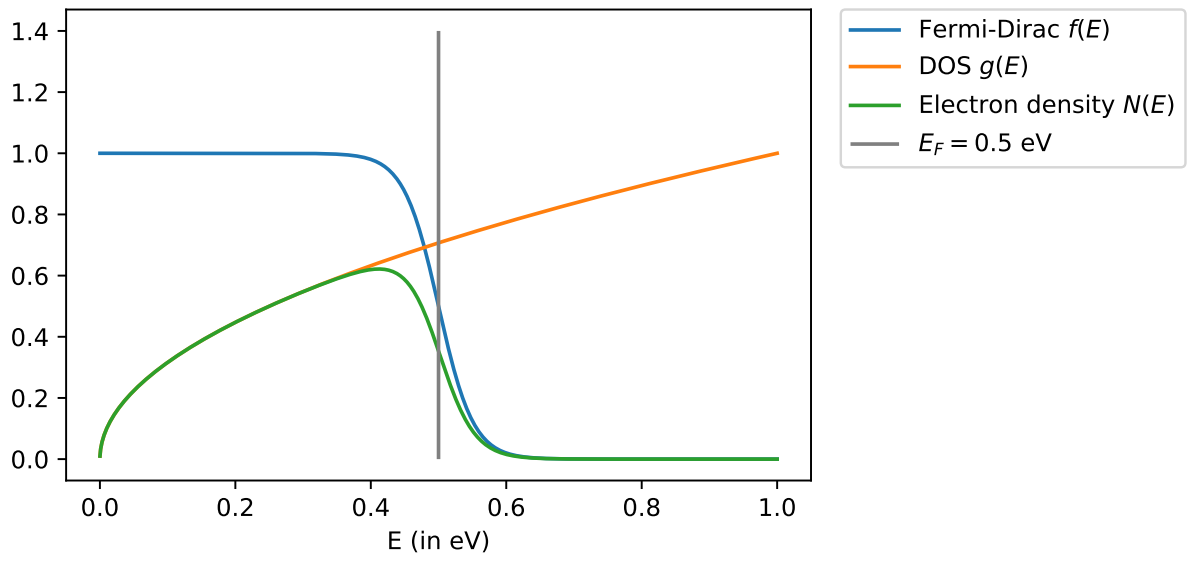
Solution (Q6)

(a) The Fermi-energy of sodium (Na) is given by:

$$\begin{aligned}
 E_F &= (0.36 \times 10^{-18} \text{ eV m}^2) \cdot n_e^{2/3} \\
 &= (0.36 \times 10^{-18} \text{ eV m}^2) \cdot (2.7 \times 10^{28} \text{ m}^{-3})^{2/3} \\
 &= (0.36 \times 10^{-18} \text{ eV m}^2) \cdot (27 \times 10^{27} \text{ m}^{-3})^{2/3} \\
 &= (0.36 \times 10^{-18} \text{ eV m}^2) \cdot (9 \times 10^{18} \text{ m}^{-2}) \\
 &= (0.36 \text{ eV}) \cdot 9 = 3.24 \text{ eV}
 \end{aligned}$$

The resulting value of $E_F = 3.24 \text{ eV}$ is of expected order when comparing with the E_F of other metals in the table.

(b) Below we show the density of states $g(E)$, the Fermi-dirac distribution $f(E)$, and the electron density $N(E) = g(E) f(E)$ as function of the energy. We used $k_B T = 25.7 \text{ meV}$ ($T = 298 \text{ K}$), and $E_F = 0.5 \text{ eV}$, but for this question the sketch does not need to be for specific parameters.



Values and formulas:

Mass of an electron: $m_e = 9.11 \times 10^{-31}$ kg

Mass of a proton: $m_p \approx 1836 m_e$

1 eV = 1.602×10^{-19} J

An atomic mass unit: 1 Dalton = 1.66×10^{-27} kg $\approx \frac{5}{3} \times 10^{-27}$ kg

Bohr magneton: $\mu_B = 9.3 \times 10^{-24}$ J/T = 5.8×10^{-5} eV/T

Joule in SI units: [J = kg m²/s²]

$h = 6.63 \times 10^{-34}$ J s = 4.14×10^{-15} eV s

$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34}$ J s = 6.582×10^{-16} eV s

$c = 3 \times 10^8$ m/s

$hc = 1240$ eV nm

Rydberg energy unit: Ry = 13.6 eV

Rydberg constant for hydrogen: $R_H = 1.0968 \times 10^7 \text{m}^{-1} \approx 1.1 \times 10^7 \text{m}^{-1}$

$m_e c^2 = 0.511$ MeV

For a wave function $\psi(x)$ with $x \in \mathbb{R}$, the expectation value of a function $f(x)$ is:

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x) |\psi(x)|^2 dx.$$

Definite integrals:

$$\begin{aligned} \int_{-\infty}^{+\infty} x^n e^{-ax^2} dx &= 0 \quad \text{for } n \text{ odd} \\ \int_{-\infty}^{+\infty} e^{-ax^2} dx &= \sqrt{\frac{\pi}{a}} \\ \int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx &= \frac{1}{2a} \sqrt{\frac{\pi}{a}} \end{aligned}$$

Particle in a box: A quantum particle in a 3D infinitely deep square well of size $L = L_x = L_y = L_z$ has wave function solutions $\psi_{n_x, n_y, n_z}(x)$ and E_{n_x, n_y, n_z} given by

$$\psi_{n_x, n_y, n_z}(x) = \sqrt{\frac{8}{L^3}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right), \quad E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$