Classwork 1 – Atomic units

Note: To solve the following problems you may use any information in the “Useful Formulae” sheet.

Atomic units make quantum-mechanical calculations simpler and less prone to mistakes. In this classwork you will practise unit conversion.

1. The electronvolt is neither an SI nor an atomic unit of energy but it is widely used in quantum mechanics. The “Useful Formulae” sheet gives the relation between the photon wavelength and its energy as $\lambda E = 1240 \text{ nm}\cdot\text{eV}$.
   
   (a) Derive this relation taking care that the physical quantities you write have not only the correct numerical values but also the correct units.
   
   (b) The light emitting diode (LED) operates by applying a potential difference across a p-n junction. When crossing the junction electrons gain energy and release it as photons. What is the minimum voltage that needs to be applied to a blue LED?
   
   Hint: The blue part of the spectrum is in the range 450–500 nm.

2. Covert hartree, $E_h$, to electronvolts.

3. Frequency $\nu$ and angular frequency $\omega$ are often mistaken one for the other because they have the same units, $s^{-1}$. To avoid the mistakes it is recommended to write the units of $\omega$ as rad/s and use $s^{-1}$ (or Hz) only for $\nu$. Following this idea of keeping a distinction between units of different physical quantities, find out the atomic units of:
   
   (a) time,
   
   (b) frequency,
   
   (c) angular frequency.

4. The “Useful Formulae” sheet gives a relation between the amplitude $F$ (in atomic units) of a monochromatic plane-polarised EM wave and its intensity $I$ in units of W/cm$^2$:

   $$ F / \frac{E_h}{e a_0} = 5.338\times10^{-9} \sqrt{I / \text{ W/cm}^2} $$

   Derive the numerical constant $5.338\times10^{-9}$.
   
   Hint: Put the square root in the above equation on the LHS and use $I = (c e a_0/2) F^2$.

International prototype of the kilogram kept at the Bureau International des Poids et Mesures near Paris. This is the only one of the seven basic SI units defined by a physical artifact rather than a natural phenomenon. There is a proposal* to redefine kilogram by referring it either to the Planck constant or the Avogadro constant. The atomic units are all based on physical constants.

The relation between photon energy $E$ and its wavelength $\lambda$ is:

1. $E = h \lambda$
2. $E = \hbar \lambda$
3. $E = \frac{hc}{\lambda}$
4. $E = \frac{\hbar c}{\lambda}$

The value of the hartree is:

1. $E_h = 27.2$ eV
2. $E_h = 13.6$ eV
3. $E_h = 24.6$ eV
4. $E_h = -13.6$ eV
The atomic unit of time is:
1. $\frac{\hbar}{E_h}$
2. $\frac{E_h}{\hbar}$
3. $\frac{E_h}{a_0}$
4. $\frac{a_0}{E_h}$

The atomic unit of frequency is:
1. $\frac{E_h}{(hc)}$
2. $\frac{E_h}{(\hbar c)}$
3. $\frac{E_h}{h}$
4. $\frac{E_h}{\hbar}$

The atomic unit of angular frequency is:
1. $\frac{E_h}{(\text{rad } \hbar)}$
2. rad $\frac{E_h}{\hbar}$
3. $\frac{E_h}{(\text{rad } \hbar)}$
4. rad $\frac{E_h}{\hbar}$

The relation between the hartree and the bohr is:
1. $E_h = \frac{e}{(4\pi \varepsilon_0 a_0^2)}$
2. $E_h = \frac{e^2}{(4\pi \varepsilon_0 a_0^2)}$
3. $E_h = \frac{e^2}{(4\pi \varepsilon_0 a_0)}$
4. $E_h = \frac{e}{(\varepsilon_0 a_0^2)}$
Classwork 2 – VUV helium lamp

Introduction
Air absorbs ultraviolet radiation at wavelengths shorter than 200 nm. Any experiments involving this radiation must be performed in vacuum and this is why the spectral range 10–200 nm (photon energies 124–6.2 eV) is called vacuum ultraviolet (VUV). The choice of VUV optics is very limited and most methods of VUV generation require sophisticated and expensive instrumentation, such as *Diamond* synchrotron at the Rutherford Appleton Laboratory.

Using an electric discharge in a noble gas offers a simple alternative, albeit limited to a few spectral wavelengths, and helium ion provides the shortest ones. Such a helium lamp is used for experiments at Imperial College. The picture below shows the lamp and the apparatus which uses the VUV radiation in one of the labs.

In the problems that follow you will need to consider the process of emission of the VUV radiation from a helium ion. You may find the “Useful Formulae” sheet helpful.
Problems

In the helium lamp an electron from the discharge impacts on a He atom, ionises it and at the same time excites it to a superposition of several states. For simplicity, let us consider only the states that are of practical importance and assume that the He\(^+\) ion immediately after the impact is left in the following superposition of states:

\[ \psi(r, t = 0) = \psi_0(r) = A \left[ 10 u_{100}(r) + 2 u_{210}(r) + u_{310}(r) \right], \]

where \(u_{nlm}(r)\) are energy eigenfunctions of the hydrogen atom.

Use the Dirac notation, e.g. \(\psi_0(r) = \langle r | \psi_0 \rangle\) and \(u_{nlm}(r) = \langle r | n \ l \ m \rangle\), in solving the following problems:

1. Find the normalisation constant \(A\).
2. Is \(\psi_0\) an eigenfunction of the parity operator?
3. What are the probabilities of finding the He\(^+\) ion in each of the following states at \(t = 0\):
   - (a) \(|1 \ 0 \ 0\rangle\),
   - (b) \(|2 \ 0 \ 0\rangle\),
   - (c) \(|2 \ 1 \ 0\rangle\),
   - (d) \(|3 \ 1 \ 0\rangle\)?
4. Assuming an infinitely heavy nucleus (i.e. the reduced mass \(m = m_e\)) calculate the energies (in atomic units) of each of the following states:
   - (a) \(|1 \ 0 \ 0\rangle\),
   - (b) \(|2 \ 1 \ 0\rangle\),
   - (c) \(|3 \ 1 \ 0\rangle\).
5. What are the expectation values in atomic units for the state \(|\psi_0\rangle\) of:
   - (a) the energy?
   - (b) the \(L^2\) operator?
   - (c) the \(L_z\) operator?
6. After \(t = 0\) the excited states can decay to the ground state emitting photons.
   - (a) Calculate the photon energies in both the atomic units and the electronvolts, and the corresponding wavelengths in nanometres.
   - (b) Considering that only a fraction of \(\psi_0\) is in the excited states and the energy expectation (see 5a) is not much above the ground state (see 4a), explain how can the photon energy (see 6a) be so large? How is the energy conserved? Clarify this issue and explain the meaning of \(\psi_0\).
Classwork 2 – VUV helium lamp

\[ \psi_0(r) = A [10 \ u_{100}(r) + 2 \ u_{210}(r) + u_{310}(r)] \]

Classwork 2 – Re: problem 1

In the Dirac notation:
1. \[ |\psi_0(r)\rangle = A (10 \langle r | 100 \rangle + 2 \langle r | 210 \rangle + \langle r | 310 \rangle) \]
2. \[ \psi_0(r) = A (10 |100\rangle + 2 |210\rangle + |310\rangle) \]
3. \[ |\psi_0\rangle = A (10 |100\rangle + 2 |210\rangle + |310\rangle) \]
4. \[ |\psi_0\rangle = A (10 |100\rangle + 2 |210\rangle + |310\rangle) \]

The orthonormality relation of the eigenstates is:
1. \[ \langle nlm | n'l' m' \rangle = \delta_{ll'} \]
2. \[ \langle nlm | n'l' m' \rangle = \delta(l - l') \]
3. \[ \langle nlm | n'l' m' \rangle = \delta_{ll'} \delta_{mm'} \]
4. \[ \langle nlm | n'l' m' \rangle = \hat{1} \]

The normalisation constant can be calculated from:
1. \[ (|\psi_0\rangle)^2 = 1 \]
2. \[ \langle \psi_0 | \psi_0 \rangle = 1 \]
3. \[ \langle \psi_0 | \psi_0 \rangle = A^2 \]
4. \[ \langle \psi_0 | \psi_0 \rangle^2 = 1 \]

The parity operator transforms an eigenvector in the following way:
1. \[ \hat{P} |n m \rangle = (-1)^l |n m \rangle \]
2. \[ \hat{P} |n l m \rangle = (-1)^{(l+1)} |n l m \rangle \]
3. \[ \hat{P} |n l m \rangle = (-1)^{n-1} |n l m \rangle \]
4. \[ \hat{P} |n l m \rangle = (-1)^{(l+1)} |n l m \rangle \]

Parity operator (inversion)
\[ \hat{P} \psi_+(\vec{r}) = \psi_-(\vec{-r}) \]
\[ \hat{P} = \hat{1} \] (unit operator)

Eigenvectors: \[ \pm |n l m \rangle \]

Eigenvectors:
\[ \psi_+ = |(1) \rangle \]
\[ \psi_- = |(-1) \rangle \]

\[ \hat{P} \psi_+(\vec{r}) = \psi_-(\vec{-r}) \]
\[ \hat{P} \psi_- (\vec{r}) = -\psi_+ (\vec{r}) \]

\[ \hat{P} |\psi_\pm \rangle = \pm |\psi_\pm \rangle \]
### Classwork 2 – Re: problem 3

The probability of finding the He\(^+\) ion in state |1 0 0\> is given by:

1. \( P_{100} = \left| \langle r | 100 \rangle \right|^2 \)
2. \( P_{100} = \langle 100 | \psi_0 \rangle \)
3. \( P_{100} = \left| \langle 100 | \psi_0 \rangle \right|^2 \)
4. \( P_{100} = \langle r | 100 \rangle \)

### Classwork 2 – Re: problem 4

The energies of the He\(^+\) ion are:

1. \( E_n = -\frac{E_h}{2} \frac{1}{n^2} \)
2. \( E_n = -E_h \frac{1}{n^2} \)
3. \( E_n = -E_h \frac{2}{n^2} \)
4. \( E_n = -E_h \frac{4}{n^2} \)

### Classwork 2 – Re: problem 5

The square of the angular momentum operator has the eigenvalues given by:

1. \( \hat{L}^2 \left| n l m \right\rangle = l(l+1)\hbar^2 \left| n l m \right\rangle \)
2. \( \hat{L}^2 \left| n l m \right\rangle = (-1)^l \left| n l m \right\rangle \)
3. \( \hat{L}^2 \left| n l m \right\rangle = m\hbar \left| n l m \right\rangle \)
4. \( \hat{L}^2 \left| n l m \right\rangle = \delta_{nm} (-1)^l \left| n l m \right\rangle \)

### Classwork 2 – Re: problem 6

The wavelength of the photon emitted in the transition |3 1 0\> → |1 0 0\> is:

1. \( \lambda_{31} = 102 \text{ nm} \)
2. \( \lambda_{31} = 30.4 \text{ nm} \)
3. \( \lambda_{31} = 122 \text{ nm} \)
4. \( \lambda_{31} = 25.6 \text{ nm} \)
Classwork 3 – Comet

Note: To solve the following problems you may use any information in the “Useful Formulæ” sheet.

When a comet passes by the Earth, sunlight heats the comet and the gases evaporate from its frozen nucleus forming the head and the tail. A water molecule dissociates and one of the hydrogen atoms is excited by the sunlight. Describe the following aspects of this excitation:

1. Show that the transition $1s \rightarrow 2s$ is not allowed, by explicitly calculating the transition dipole moment between the two states for the polarization:
   - (a) parallel to the $z$ axis,
   - (b) parallel to the $x$ or $y$ axis.

2. Estimate the order of magnitude of the excitation rate (per second) of the atom by considering its strongest transition, $1s \rightarrow 2p$, in the following steps:
   - (a) Substitute the typical transition dipole moment, $-ea_0$, into the relevant Einstein coefficient.
   - (b) Combine the result from part (a) with the spectral density of black body radiation (Planck’s law) to obtain the transition rate for an atom exposed to isotropic sunlight illumination.
   - (c) Take into account that the sunlight comes to the comet only from a small solid angle: the (linear) angular diameter of the Sun is 0.5º.

3. Calculate the de-excitation rate of the reverse transition, $2p \rightarrow 1s$. How does it compare with the excitation rate? What fraction of the hydrogen atoms in the comet head will be in the excited state at any time?

4. Check the units of the results in points 2 and 3.
Classwork 3 – How to calculate selection rules?

Comet

1. Show that the transition $1s \rightarrow 2s$ is not allowed by explicitly calculating the electric dipole moment between the two states for the radiation polarization:
   - (a) parallel to the $z$ axis,
   - (b) parallel to the $x$ or $y$ axis.

Classwork 3 – Re: problem 1(a)

For $\varepsilon || z$,

For $\varepsilon || r$, $\varepsilon \cdot r$

1. $r \sin \theta \sin \varphi$
2. $r \sin \theta \cos \varphi$
3. $r \cos \theta \sin \varphi$
4. $r \cos \theta \cos \varphi$

Classwork 3 – Hydrogenic wavefunctions

Einstein coefficient for absorption depends on the transition dipole moment $\mu$ in the following way:

1. $B_{12} = \frac{\mu^2}{4\pi\varepsilon_0 \hbar}$
2. $B_{12} = \frac{\pi\varepsilon_0}{\varepsilon_0 \hbar}$
3. $B_{12} = \frac{\pi\mu^2}{\varepsilon_0 \hbar^2}$
4. $B_{12} = \frac{\mu^2}{4\pi\varepsilon_0 \hbar^2}$
### The spectral density of black body radiation

1. \( \rho(\omega) = \frac{h\omega^3}{\pi^2c^3} e^{\frac{k\omega}{c}T} \)
2. \( \rho(\omega) = \frac{h\omega^3}{\pi^2c^3} e^{\frac{k\omega}{c}T} \)
3. \( \rho(\omega) = \frac{h\omega^3}{\pi^2c^3} e^{\frac{k\omega}{c}T} \)
4. \( \rho(\omega) = \frac{h\omega^3}{\pi^2c^3} e^{\frac{k\omega}{c}T} \)

### The temperature of Sun’s photosphere

1. 4800 K
2. 6800 K
3. **5800 K**
4. 7800 K

### The solid angle subtended by the Sun

1. \( \Omega = 2\pi\delta \)
2. \( \Omega = \pi\delta^2 \)
3. \( \Omega = \pi\delta^2 \)
4. \( \Omega = \delta^2 \frac{\pi}{4} \)

### In this problem, the processes responsible for the de-excitation are:

1. equally spontaneous and stimulated emissions
2. mainly stimulated emission
3. **mainly spontaneous emission**
4. mainly absorption
Classwork 4 – Negative ion

Note: To solve the following problems you may use any information in the “Useful Formulae” sheet.

It is possible to form the negative ion of hydrogen, H\(^-\), by attaching an extra electron to the hydrogen atom.

1. Deduce the spin state of the ground state of the H\(^-\) ion by considering indistinguishability of the two electrons.

2. What is the energy required to remove both electrons from the H\(^-\) ion within the independent particle approximation?

3. Use first order perturbation theory to estimate a more accurate value of this energy as follows:
   
   (a) recall that Handout 5 evaluates the Coulomb integral as \( J = \frac{5}{8} \frac{e^2}{4\pi \varepsilon_0} \frac{Z}{a_0} \);
   
   (b) express this result in terms of \( Z \) and the Hartree energy, \( E_h \);
   
   (c) calculate the value of \( J \) in eV.

4. Sketch appropriate energy diagrams and comment upon what your results in parts 1–3 say about the stability of this ion (in fact this ion is stable because the experimental value of the energy required to remove both electrons is 14.4 eV).

Tandem accelerator used for many years at Daresbury Laboratory. The diagram shows the principle of a tandem van de Graaff accelerator. Negatively charged ions from an ion source at ground potential are accelerated towards a terminal at high positive potential in the centre, where gas or a thin foil removes two or more electrons from the ions, which then become positively charged and repelled towards the grounded electrode \((V = 0)\). Electric charge is transported on a belt from the ground to the terminal and as a consequence of the charge accumulation, the potential increases. The high voltage \((V = +5 \text{ MV})\) is insulated from the ground by high pressure gas, normally SF\(_6\).

http://nobelprize.org/nobel_prizes/physics/articles/kullander/
Classworks for Applications of Quantum Mechanics, Leszek Frasiński, Jan-Feb 2012

Classwork 4: Negative ion

In the ground state of He,

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} \chi_{10}(1,2)$$

1. $$(u_{1s}(r_1)u_{1s}(r_2) - u_{1s}(r_2)u_{1s}(r_1)) \chi_{10}(1,2)$$
2. $$(u_{1s}(r_1)u_{1s}(r_2) - u_{1s}(r_2)u_{1s}(r_1)) \chi_{110}(1,2)$$
3. $$(u_{1s}(r_1)u_{1s}(r_2) + u_{1s}(r_2)u_{1s}(r_1)) \chi_{00}(1,2)$$
4. $$(u_{1s}(r_1)u_{1s}(r_2) + u_{1s}(r_2)u_{1s}(r_1)) \chi_{110}(1,2)$$

In terms of single-electron spin functions, the singlet state

$$\chi_{10}(1,2) = \frac{1}{\sqrt{2}} \left( \chi_1(1) \chi_2(2) - \chi_2(1) \chi_1(2) \right)$$

1. $$(\chi_1(1) \chi_2(2) - \chi_2(1) \chi_1(2))$$
2. $$(\chi_1(1) \chi_2(2) - \chi_2(1) \chi_1(2))$$
3. $$(\chi_1(1) \chi_2(2) + \chi_2(1) \chi_1(2))$$
4. $$(\chi_1(1) \chi_2(2) + \chi_2(1) \chi_1(2))$$

Classwork 4 – Re: problem 2

Atomic number for the H$^-$ ion:

1. $Z = 3$
2. $Z = 4$
3. $Z = 2$
4. $Z = 1$

Classwork 4 – Re: problem 2

Within IPA, to remove both electrons from H$^-$ we need:

1. $27.2$ eV
2. $13.6$ eV
3. $108.8$ eV
4. $54.4$ eV

Classwork 4 – Re: problem 4

To have a stable H$^-$ ion it is sufficient that the energies in the ground state satisfy:

1. $E(H^-) < E(H^+)$
2. $E(H^-) > E(H^+)$
3. $E(H^-) < E(H)$
4. $E(H^-) > E(H)$
Classwork 1 – Solutions

1. (a) \[ E = \frac{\hbar c}{\lambda} \]
   \[ \lambda E = \frac{\hbar c}{\frac{\hbar}{m_s} \frac{c}{m_s} \frac{J_m}{eV 10^9 \text{nm}}} \]
   \[ \lambda E = \frac{\hbar/(Js)}{e/C} \frac{c/m_s}{10^9 \text{eV nm}} \]
   \[ \lambda E = 1240 \text{ eV nm} \]

(b) \[ E_{\text{max}} = 500 \text{ nm} \]
   \[ E_{\text{min}} = \frac{1240 \text{ nm eV}}{500} = 2.48 \text{ eV} \]
   \[ U_{\text{min}} = E_{\text{min}} / q = 2.48 \text{ eV} / e = 2.48 \text{ V} \]

2. \[ E_h = \frac{\hbar^2}{m_e a_0^2} = \frac{(\hbar/(Js))^2}{(m_e/kg)(a_0/m)^2} \frac{J^2 s^2}{kg m^2} \]
   \[ E_h = \frac{(\hbar/(Js))^2}{(m_e/kg)(a_0/m)^2(e/C)} \text{ eV} \]
   \[ J = C V = \frac{C}{e} \text{ eV} \]
   \[ E_h = 27.2 \text{ eV} \]

3. (a) a.u. of time = \[ \frac{h}{E_h} \]

(b) a.u. of \[ \nu = 1 / (\text{a.u. of time}) = E_h / h \]

(c) \[ \omega = 2\pi \nu = 2\pi \text{ rad} \times \nu \]
   \[ \frac{\omega}{\text{rad} E_h / h} = 2\pi \frac{\nu}{E_h / h} \]
   \[ \therefore \text{a.u. of } \omega = \text{rad} E_h / h \]
4. \[ \frac{F}{E_h \sqrt{2 \pi a_o}} = \frac{e a_o}{E_h} \sqrt{\frac{2}{c E_0}} \sqrt{\frac{W}{c m}} = \frac{e a_o}{E_h} \sqrt{\frac{8 \pi E_h a_o}{c e^2}} \frac{100}{\sqrt{m}} \]

\[ I = \frac{e^2}{2} \frac{E_0}{4 \pi e_h a_0} \]

\[ W = J/s \]

\[ I = \frac{2 e^2}{2 \pi a_o} \frac{J}{m^2 s} = 200 \left( \frac{2 \pi \left( a_o/m \right)^3}{(c/\omega)^5 (E_h/J)} \right) \]

\[ = 200 \sqrt{\frac{2 \pi \times (5.292 \times 10^{-11})^3}{299.8 \times 10^6 \times 4.360 \times 10^{-19}}} = 5.338 \times 10^{-9} \]
Classwork 2 – Solutions

1. \[ \langle \psi_0 | \psi_0 \rangle = A^2 \left( |10\rangle \langle 10| + 2 |21\rangle \langle 21| + |31\rangle \langle 31| \right) \]
   \[ x \left( |10\rangle \langle 10| + 2 |21\rangle \langle 21| + |31\rangle \langle 31| \right) \]
   \[ = A^2 (100 + 4 + 1) = 105 A^2 \]
   \[ A = \frac{1}{\sqrt{105}} \]

2. \[ \hat{\mathbf{P}} | n \ell m \rangle = (-1)\ell | n \ell m \rangle \]
   \[ \hat{\mathbf{P}} | \psi_0 \rangle = A \left( |10\rangle \langle 10| + 2 |21\rangle \langle 21| + |31\rangle \langle 31| \right) \]
   \[ = A \left( |10\rangle - |21\rangle - |31\rangle \right) \neq | \psi_0 \rangle \]
   \( N_\theta \), it is not.

3. (a) \[ P_{100} = | \langle 100 | \psi_0 \rangle |^2 = \left| \frac{10}{\sqrt{105}} \right|^2 = \frac{100}{105} \]
   (b) \[ P_{200} = | \langle 200 | \psi_0 \rangle |^2 = 0 \]
   (c) \[ P_{210} = | \langle 210 | \psi_0 \rangle |^2 = \left| \frac{2}{\sqrt{105}} \right|^2 = \frac{4}{105} \]
   (d) \[ P_{310} = | \langle 310 | \psi_0 \rangle |^2 = \left| \frac{1}{\sqrt{105}} \right|^2 = \frac{1}{105} \]

4. \[ E = 2, \quad E_n = -E_h \frac{2}{n^2} \]
   (a) \[ E_1 = -2E_h \]
   (b) \[ E_2 = -E_h / 2 \]
   (c) \[ E_3 = -\frac{2}{9} E_h \]
(b) The meaning of $\psi_0$ is that the numerical coefficients in the assumed superposition give us probability amplitudes of finding the He$^+$ ion in a given energy eigenstate. Nearly 95% of the ions are found in the ground state (see answer 3a) and the energy expectation is heavily weighted towards the energy of this state.

Individual photons, however, are emitted only from the ~5% of the excited states (see answers 3c and 3d). The photon energy is so large because only a small fraction of the whole ion population emits these photons. The photons are emitted as whole quanta of energy and in a long run, when we detected many photons, the photon energy averaged over the whole population tends to the energy difference between the energy expectation and the ground state energy.

On a short run, however, when we detect only a few photons, their average energy may deviate from the expectation-to-ground energy difference. This does not mean the energy is not conserved, it only means that the energy of state $|\psi_0\rangle$ is uncertain because it is in a superposition of states of different energy eigenvalues.

\[ \langle \psi_0 | \hat{H} | \psi_0 \rangle = P_{100} E_1 + P_{210} E_2 + P_{310} E_3 = \]
\[ = -\left( \frac{100}{105} \times 2 + \frac{4}{105} \times \frac{1}{2} + \frac{1}{105} \times \frac{2}{9} \right) E_h = \]
\[ = - \frac{100 + 1 + 0.1}{105} \times 2 E_h = - \frac{101.1}{105} \times 2 E_h = -1.926 E_h \]

\[ \langle \psi_0 | \hat{L}_z^2 | \psi_0 \rangle = \]
\[ = P_{100} 0(0+1) \hbar^2 + P_{210} 1 \times 2 \hbar^2 + P_{310} 1 \times 2 \hbar^2 = \]
\[ = \left( \frac{4}{105} \times 2 + \frac{1}{105} \times 2 \right) \hbar^2 = \frac{10}{105} \hbar^2 \]

\[ \langle \psi_0 | \hat{L}_z^2 | \psi_0 \rangle = 0 \text{ because every } m = 0 \]

6. (a) \[ E_1 = E_2 - E_1 = \]
\[ = -E_h/2 - (-2E_h) = \frac{3}{2} E_h = 30.4 \text{ nm} \]
\[ \lambda_{21} = \frac{1240 \text{ nm} \cdot \text{eV}}{40.8 \text{ eV}} \]
\[ = 29.6 \text{ nm} \]

\[ E_3 = E_3 - E_1 = \]
\[ = -\frac{2}{9} E_h - (-\frac{18}{9} E_h) = \frac{16}{9} E_h = 48.4 \text{ eV} \]

(b) The meaning of $\psi_0$ is that the numerical coefficients in the assumed superposition give us probability amplitudes of finding the He$^+$ ion in a given energy eigenstate. Nearly 95% of the ions are found in the ground state (see answer 3a) and the energy expectation is heavily weighted towards the energy of this state.

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Classwork 3 – Solutions

1. \( \mu = -e \langle 2s | \mathbf{\varepsilon} \cdot \mathbf{r} | 1s \rangle \)

(a) \( \mathbf{\varepsilon} \parallel z \) \( \mathbf{\varepsilon} \cdot \mathbf{r} = r \cos \theta \)

\[
\mu = -e \int_0^\infty dr \, r^2 R_{20}(r) R_{10}(r) \int_0^\pi d\theta \sin \theta \gamma_{00}(\theta, \phi) \cos \theta \gamma_{00}(\theta, \phi) \int_0^{2\pi} d\phi \frac{2\pi}{\sqrt{4\pi}} \frac{1}{\sqrt{4\pi}} \frac{1}{2\pi} \\
\mu \propto \int_0^\pi d\theta \sin \theta \cos \theta = \int_0^\pi d\theta \frac{1}{2} \sin(2\theta) = 0
\]

(b) \( \mathbf{\varepsilon} \parallel x \) \( \mathbf{\varepsilon} \cdot \mathbf{r} = r \sin \theta \cos \phi \)

\[
\mu \propto \int_0^\pi d\theta \sin^2 \theta \int d\phi \cos \phi = 0
\]

(c) \( \mathbf{\varepsilon} \parallel y \) \( \mathbf{\varepsilon} \cdot \mathbf{r} = r \sin \theta \sin \phi \)

\[
\mu \propto \int_0^{2\pi} d\phi \sin \phi = 0
\]

2. (a) From "Useful Formulae" Einstein coefficient for absorption

\[
\beta_{12} = \frac{\pi \alpha^2}{E_0} = \frac{\pi \alpha^2}{E_0} = \frac{4\pi \alpha^2}{\hbar^2}
\]

(b) From lectures, transition rate for isotropic illumination

\[
W = \beta_{12} \rho(\omega) = 4\pi^2 \frac{E_h \alpha^2}{\hbar^2} \frac{\hbar \omega^3}{\pi^2 \mathcal{C}^3} \frac{1}{e^{\hbar \omega/kT} - 1}
\]

fine structure constant

\[
W = 4 \frac{E_h}{\hbar} \left( \frac{\alpha}{E_h} \frac{\hbar \omega}{E_h} \right)^3 \frac{1}{e^{\hbar \omega/kT} - 1} \approx 4.6 \frac{1}{5}
\]

\[
\frac{1}{240 s} \frac{1}{137} \frac{3}{8} \frac{T_{\text{sun}} = 5800 K}{K} \frac{1}{38} \frac{K}{E_h} = 3.17 \times 10^{-6} K^{-1}
\]

\[
\frac{\hbar \omega}{E_h} = \frac{E_{2p} - E_{1s}}{E_h} = -\frac{1}{2} \left( \frac{1}{22} - \frac{1}{12} \right) = \frac{3}{8}
\]
(c) Transition rate at the comet \( W_C = \frac{\Omega}{4\pi} W \)

Solid angle subtended by the Sun \( \Omega = \pi \frac{D^2}{4} \)

Linear angular diameter of the Sun \( \delta = 0.5^\circ = 0.5 \times \frac{\pi}{360} \text{ rad} \)

\[
W_C = \frac{1}{4\pi} \frac{\pi^2}{4} \frac{D^2}{360^2} W = \frac{\pi^2}{16 \times 360^2} W = 4.76 \times 10^{-6} W = 2.2 \times 10^{-5} \frac{1}{5} = 1.9 \text{ / day}
\]

The sunlight excites the hydrogen atom about twice a day.

3. The de-excitation rate is dominated by the Einstein coefficient for spontaneous emission:

\[
A_{21} = \frac{\hbar \omega^3}{n^2 c^3} B_{21}, \quad \text{where} \quad B_{21} = \frac{\pi M^2}{E_0 \hbar^2} = \frac{4\pi^2 \alpha^3 a_0^3}{\hbar^2} = 4\pi^2 \frac{E_h a_0^3}{\hbar^2}
\]

\[
A_{21} = \frac{\hbar \omega^3}{n^2 c^3} 4\pi^2 \frac{E_h a_0^3}{\hbar^2} = 4 \frac{E_h}{\hbar} \left( \frac{\alpha}{\hbar c} \right)^3 (\hbar \omega)^3 = \frac{\alpha}{E_h} \omega^3
\]

\[
= 4 \frac{E_h}{\hbar} \left( \frac{\alpha}{E_h} \omega \right)^3 = \frac{4}{24 \times \frac{1}{37} \times \frac{3}{8}} = 3.39 \times 10^9 \frac{1}{5}
\]

The de-excitation rate is over 14 orders of magnitude faster than the excitation rate. Less than \( 10^{-14} \) atoms in the comet head will be in the excited state at any time.

4. The final formulae in parts 2 and 3 are in a form that allow checking units at a glance.
Classwork 4 – Solutions

1. \((p^+, 2e^-)\), similar reasoning to He:
   - total \(\psi(\vec{r}_1, \vec{r}_2) = \Psi(\vec{r}_1, \vec{r}_2) \chi_{SM}^{(1,2)}\)
     must be antisymmetric (e\(^-\) are fermions)
   - spatial part, ground state 1S\(^2\)
     \(\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left( \chi_{1S}(\vec{r}_1) \chi_{1S}(\vec{r}_2) \pm \chi_{1S}(\vec{r}_2) \chi_{1S}(\vec{r}_1) \right)\)
     vanishes for the antisymmetric (\(-\)) case
   - only symmetric (\(+\)) is permissible

\(\Rightarrow\) the spin state must be antisymmetric (singlet):
\(\chi_{00}^{(1,2)} = \frac{1}{\sqrt{2}} \left( \chi_+^{(1)} \chi_-^{(2)} - \chi_-^{(1)} \chi_+^{(2)} \right)\)
or
\(|SM\> = |00\> = \frac{1}{\sqrt{2}} \left( |+\> - |-\> \right)\)

2. In IPA \(\text{H}^-=2\text{H}\), each with ionisation energy \(E_h/2 = 13.6\text{ eV} \quad (Z=1)\)
   \(\therefore\) total binding energy \(E_h = 27.2\text{ eV}\)

3. (b) from Useful Formulae: \(E_h = \frac{e^2}{4\pi \varepsilon_0 a_0}\)
   \(\therefore\) \(J = \frac{5}{8} E_h 2\)
   (c) \(J = \frac{5}{8} \times 27.2\text{ eV} \times 1 = 17\text{ eV}\)

4. IPA \(\text{H}^-\) Perturb. \(\text{H}\) atom
   - real \(\text{H}^-\)
   - In the 1st order \(E(\text{H}^-) > E(\text{H})\)
     \(\Rightarrow\) \(\text{H}^-\) unstable & decays to \(\text{H} + e^-\)

   - \(E(\text{H}) < E(\text{H})\)
     \(\Rightarrow\) \(\text{H}^-\) stable