(P.1)

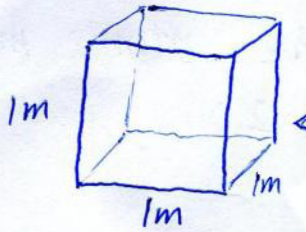
Solution by Leung Hing Shing.

SQ1. Suppose you are a physicist in 1910's. To understand the structures of atoms, knowing the sizes of atoms are fundamental questions. The question is:

How to estimate the size of an atom?

Aim: to calculate the radius of a carbon atom.

① Information given:

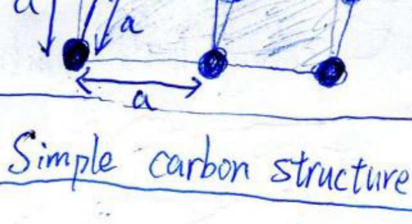


$1\,m^3$ of diamond
weight: 3.5×10^3 kg

a carbon atom: relative atomic mass of 12.0

② Simplification / assumption.

To make the calculation easier, we assume the carbon atoms are arranged in "cubic structure", in place of "ABC-A cubic close packing" (this is only a jargon)



Carbon nucleus

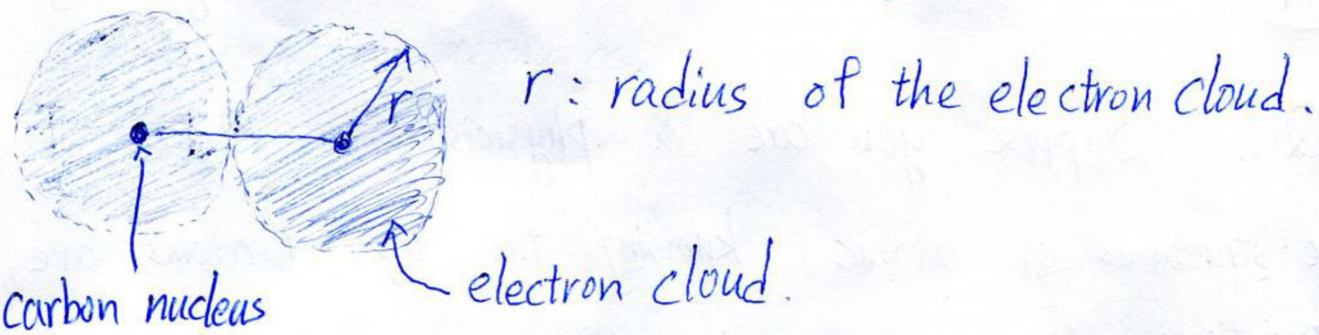
I mean this

Simple carbon structure (cubic)

Real carbon strusture (ABCA)

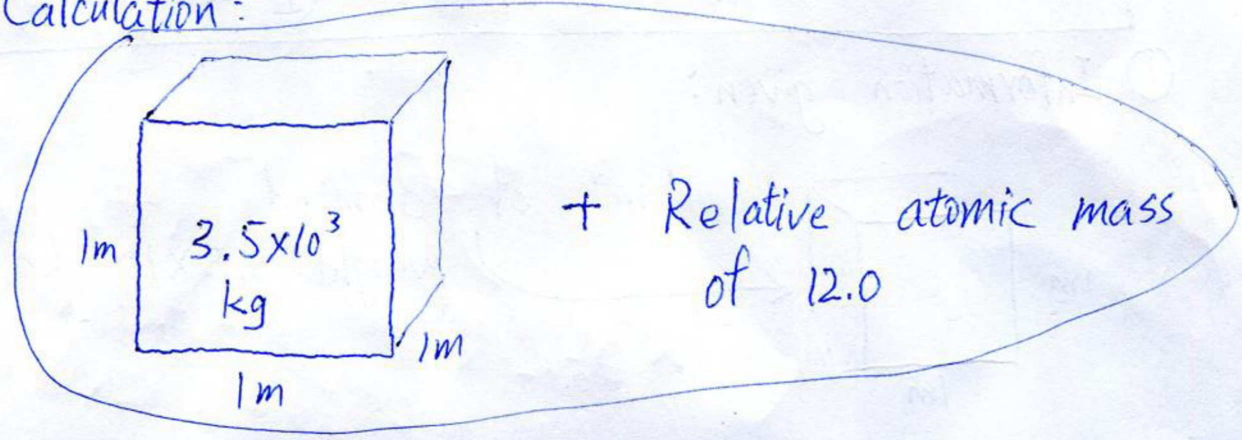
P.2

The carbon nucleus is surrounded by electron cloud.



And also, we assume the radius of an atom is the radius of this electron cloud (defining the radius of an atom).

③ Calculation:



- To calculate the number of carbon atoms in this one 1 m^3 box, (3.5×10^3 kg) and (12.0) are the numbers we want.

The number of mole of carbon atoms in 1 m^3 box

$$= \frac{(3.5\times10^3)\ \text{kg}}{\left(\frac{12}{1000}\right)\text{kg mol}^{-1}} = 291666.666\ldots\ \text{mol}$$

- To calculate the volume of a electron cloud (an a we divide the 1m^3 box into many many many carbon atoms.

Therefore, the volume of a electron cloud

$$\approx \frac{1\,m^3}{(\underset{\text{no. of mole of Carbon atoms}}{291666.666\ldots})\ (\underset{\text{Avogadro's number}}{6.02\times10^{23}})}$$

$\approx 5.70 \times 10^{-30}\ m^3$

$= 5.70\ \text{Å}^3 \quad (1\ \text{Å} = 10^{-10}\ m)$

The volume of the electron cloud is 5.70 Å^3, then we can find the radius of the electron cloud.

$$\text{Volume} = 5.70\ \text{Å}^3$$

$$= \frac{4}{3}\pi r^3$$

$$\Rightarrow \boxed{r \approx 1.108\ \text{Å}}$$

or $1.108 \times 10^{-10}\ m$

Under our assumptions, we calculate the radius of a carbon atom to be 1.108 Å. Looking for the radius of a carbon atom, it turns out to be 1.70 Å. (not far away).

Sources of error:

① Incorrect (but good) assumption of a simplified carbon structure

② Definition of radius in the electron cloud model could be different from the radius searched from the internet.

Please remember the size of an atom is of the order of Å (10^{-10} m).

SQ 2.

(P.4)

Aim: to know the typical values constantly used in quantum mechanics.

(a) $h = 6.626 \times 10^{-34}\ \mathrm{Js} = 4.136 \times 10^{-15}\ \mathrm{eVs}$ (Planck's constant)

$\hbar = 1.055 \times 10^{-34}\ \mathrm{Js} = 6.582 \times 10^{-16}\ \mathrm{eVs}$ $\left(\frac{h}{2\pi}\right)$

★ At least memorize the order of magnitude of h since it helps you estimate the "size" of a quantum system. A simple example is the energy of a photon. What is the energy of a X-ray photon (3×10^{16} Hz)? You can then instantly tell me that the energy is 100 eV, which is of very high energy.

$\uparrow$

$\left(E = hf \approx (4 \times 10^{-15}\ \mathrm{eVs})(3 \times 10^{16}\ \mathrm{s}^{-1})\right)$

(b)(i)
$$\frac{\hbar^2}{m_e} = \frac{(6.582 \times 10^{-16})^2 (\mathrm{eV})^2 \mathrm{s}^2}{\left(\frac{E_e}{c^2}\right)} = \frac{(6.582 \times 10^{-16})^2 \quad (\mathrm{eV})^2\,\mathrm{s}^2}{\left(\frac{0.511 \times 10^6\ \mathrm{eV}}{(3 \times 10^8)^2\ \mathrm{m}^2\,\mathrm{s}^{-2}}\right)}$$

$\uparrow$ electron mass

E_e: rest energy of electron

c: speed of light

$$= (7.63 \times 10^{-20})\ \mathrm{eV\,m}^2$$

$1\mathrm{m} = 10^{10}$ Å $\longrightarrow$ $= (7.63 \times 10^{-20})\ \mathrm{eV}\ (10^{10}\ \text{Å})^2$

$$= 7.63\ \mathrm{eV}\ \text{Å}^2$$

(ii) We know that potential energy of two interacting electrons can be writen as $V = \frac{e^2}{4\pi\varepsilon_0 r}$ or $\frac{e^2}{4\pi\varepsilon_0} = rV$ (in eV Å)

We then know $\frac{e^2}{4\pi\varepsilon_0}$ is in units of eV Å

Putting in numbers: $\frac{e^2}{4\pi\varepsilon_0} = \frac{(1.602 \times 10^{-19})^2}{4\pi(8.854 \times 10^{-12})}$ J m

$$= 2.308 \times 10^{-28}\ \mathrm{J\,m}$$
$$= 2.308 \times 10^{-28}\ (6.242 \times 10^{18}\ \mathrm{eV})(10^{10}\ \text{Å})$$
$$\approx 14.4\ \mathrm{eV}\ \text{Å}$$

(c) We can estimate the energy of an electron confined to an atom
.5 using dimensional analysis.

Given the energy of an electron confined to an atom (E) (in eV) depends on $\left(\frac{\hbar^2}{m_e}\right)$ (in eV $\mathring{A}^2$) and radius of a carbon atom r (in $\mathring{A}$ only, what is the relation between these quantities?

	E	$\frac{\hbar^2}{m_e}$	r
List the dimensions of the variables :	eV	eV $\mathring{A}^2$	$\mathring{A}$

match the dimensions :

$$\{E\} = \left\{\left(\frac{\hbar^2}{m_e}\right)^a r^b\right\}$$

$$\{eV\} = \{eV^a \mathring{A}^{2a} \mathring{A}^b\} = \{eV^a \mathring{A}^{2a+b}\}$$

$$\begin{cases} a=1 \\ 2a+b=0 \end{cases} \Rightarrow \begin{cases} a=1 \\ b=-2. \end{cases}$$

We can propose that $\boxed{E \propto \frac{\hbar^2}{m_e r^2}.}$ (This is the relation we want)

To give a concrete number let $E_0 = \frac{\hbar^2}{m_e r^2}$, and let's use this number the estimated the energy required.

$$E_0 = \frac{(\hbar^2/m_e)}{r^2}$$

$$= \frac{(7.63)\ eV\ \mathring{A}^2}{(1.108)^2\ \mathring{A}^2}$$

$$\approx 6.22 eV$$

☆ The important message here is the energy to confine a electron in an atom is of the order of eV.

Atomic Orbital Ionization Energies, eV

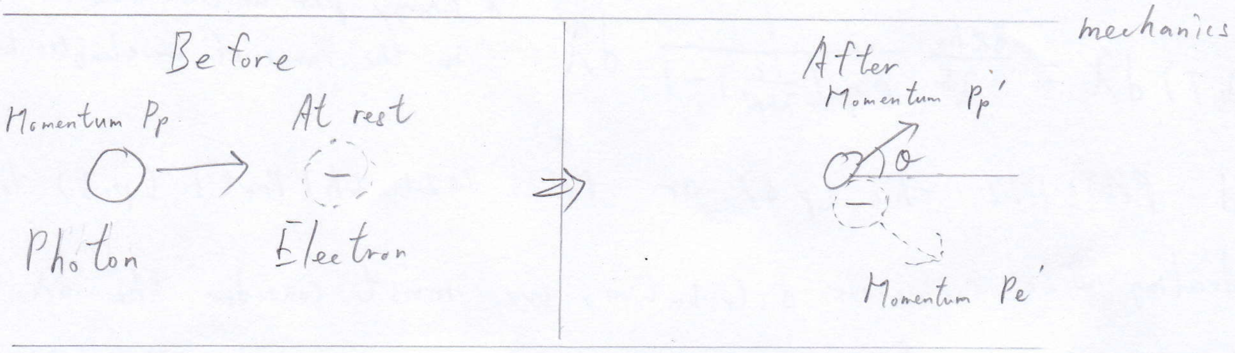
Atom	1s	2s	2p	3s	3p	4s	4p
H	13.6						
He	24.5						
Li		5.45					
Be		9.30					
B		14.0	8.30				
C		19.5	10.7				
N		25.5	13.1				
O		32.3	15.9				
F		46.4	18.7				
Ne		48.5	21.5				
Na				5.21			
Mg				7.68			
Al				11.3	5.95		
Si				15.0	7.81		
P				18.7	10.2		
S				20.7	11.7		
Cl				25.3	13.8		
Ar				29.2	15.9		
K						4.34	
Ca						6.07	
Zn						9.42	
Ga						12.6	5.95
Ge						15.6	7.56
As						17.6	9.05
Se						20.8	10.8
Br						24.0	12.5
Kr						27.5	14.3

	3d	4s	4p
Sc	4.71	5.70	3.22
Ti	5.58	6.07	3.35
V	6.32	6.32	3.47
Cr	7.19	6.57	3.47
Mn	7.93	6.82	3.59
Fe	8.68	7.07	3.72
Co	9.42	7.32	3.84
Ni	10.0	7.56	3.84
Cu	10.7	7.69	3.97

These are one-electron ionization energies of the valence orbitals calculated by finding the average energies of both the ground-state and ionized-state configurations. (Harry Gray, “Electrons and Chemical Bonding,” Benjamin, 1964, Appendix)

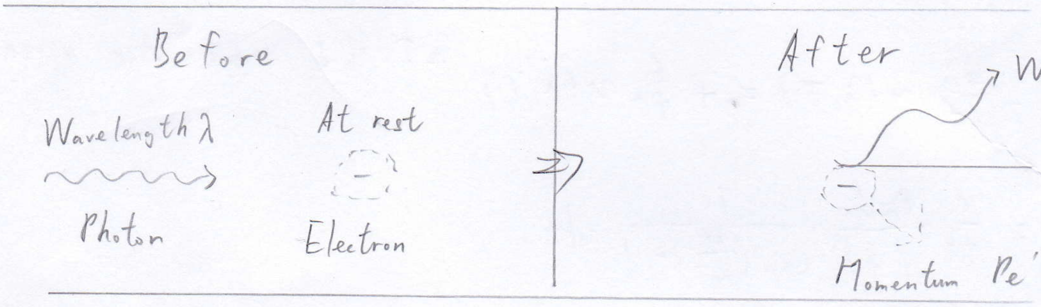
SQ3 References: Wiki, PHYS 1122 ch6.5 (p.36-40)

First, assume we know nothing about wave and consider secondary school mechanics:



We know that $\boxed{P_p > P_p'}$! The momentum of incident photon is larger!

Now consider photon as a EM Wave:



What is the relation between momentum P and wavelength λ?

$$\boxed{\text{De Broglie Wavelength (Matter Wave)}: pc = hf \Rightarrow p = \frac{h}{\lambda} \quad (E = hf)}$$

As $P_p > P_p'$, $\boxed{\lambda' > \lambda}$! The wavelength of scattered photon is longer!

By conservation of energy and momentum, we can prove that

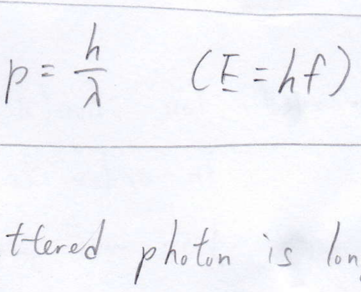
$$\boxed{\text{Compton scattering}: \lambda' - \lambda = \frac{h}{m_e}(1 - \cos\theta)}$$

*m_e is electron rest mass
See PHYS1122 ch6.5

But wait, how can we measure the wavelength λ?

Recall the Young's (or other multiple slit experiment) double slits experiment, we have $\boxed{d\sin\theta = n\lambda.}$

The diffraction is explained by $\boxed{\text{waves interference.}}$



As a result we can measure the wavelength using diffraction grating.

Thus the shifted wavelength is known.

∴ The wave property of light is involved.

SQ4

Planck's formula:

$$u(\lambda,T)\,d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right)-1}\,d\lambda$$

* Energy per unit volume at temperature T in the range of wavelengths between λ and $\lambda+d$

Read PHYS 1122 ch6 (p.6) or PHYS 3021 ch1 Part 1 (p.3) for a graph.

In dealing with continuous distribution, we must consider the $d\lambda$ carefully.

$\because\ c = f\lambda \Rightarrow \lambda = \frac{c}{f}$

$\therefore\ d\lambda = -\frac{c}{f^2}df$

We define $u(\lambda,T)\,d\lambda = -u(f(\lambda),T)\,df$, the minus sign is to indicate that $\lambda\uparrow\ f\downarrow$ and vice versa.

$$\Rightarrow u(f,T) = -\frac{d\lambda}{df}u(\lambda,T) = +\frac{c}{f^2}u(\lambda,T)$$

$$\therefore u(f,T)\,df = \frac{c}{f^2}\frac{8\pi hc}{\left(\frac{c}{f}\right)^5}\frac{1}{\exp\left(\frac{hf}{k_BT}\right)-1}\,df$$

$$= \frac{8\pi f^2}{c^3}\frac{hf}{\exp\left(\frac{hf}{k_BT}\right)-1}\,df$$

Remark 1: You should understand the relation between the original and new variable in order to make the sign right. e.g. if you do not let $u(\lambda,T)\,d\lambda = -u(f,T)\,df$, you will get an extra negative sign which makes your equation unphysical.

Remark 2: Another point of view of introducing the minus sign is considering integration.

Suppose we integrate from λ_0 to λ_1 $\quad \int_{\lambda_0}^{\lambda_1} u(\lambda,T)\,d\lambda$ where $\lambda_1 > \lambda_0$.

The result will be some POSITIVE number,

If we now change the variable from λ to f, and do the corresponding integral.

$\int_{f_0}^{f_1} u(f,T)\,df$, where $f_0 > f_1$ as $\lambda = \frac{c}{f}$.

The result will be some NEGATIVE number, which is not physical.

As a result, we introduce a minus sign.

$$\int_{f_0}^{f_1} -u(f,T)\,df = \int_{f_1}^{f_0} u(f,T)\,df$$

This time we get a POSITIVE number.