Departamento de Fisica .UBAexactas

ATTOSECOND PHYSICS



UNIT IV SYSTEM OF UNITS: HARTREE ATOMIC UNITS

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HARTREE ATOMIC UNITS



The atomic units system is used in atomic physics for its simplicity.

The atomic unit of mass is the electron mass:

 $m_e = 9.11 \times 10^{-31} \text{kg}$

The atomic unit of charge is the electron charge: $e = 1.602 \times 10^{-19} C$

The atomic unit of length is the Bohr radius:

 $a_0 = 5.29 \times 10^{-11} \text{ m}$

The atomic unit of angular momentum:

 $h = \frac{h}{2\pi} = 1.05 \times 10^{-34} \text{ J.s}$

According to the Bohr's model, the condition for mechanical stability is:

(attraction force)
$$\frac{e^2}{4\pi\varepsilon_0 r^2} = \frac{m_e v^2}{r}$$
 (centrifugal force)

HARTREE ATOMIC UNITS (cont.)



Besides, the angular momentum is: $L = m_e v r = n\hbar \implies v = \frac{n\hbar}{m r}$

$$\frac{e^2}{4\pi\varepsilon_0 r^2} = \frac{m_e n^2 \hbar^2}{r m_e^2 r^2} \Rightarrow r_n = \frac{4\pi\varepsilon_0 n^2 \hbar^2}{m_e e^2} \quad \text{radii of Bohr's orbits}$$

$$a_0 = r_1 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 4\pi\varepsilon_0 = 1 \Rightarrow \varepsilon_0 = \frac{1}{4\pi} = 8.85 \times 10^{-12} \frac{\text{C}^2\text{s}^2}{\text{m}^3\text{kg}}$$

We can derive other constants of nature like the speed of light

Fine structure
$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} = \frac{1}{137.036}$$
 (non-dimensional)
 $\Rightarrow c = 137.036$

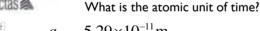
How much is a speed of I a.u.?

$$v_0 = 1 = \frac{c}{137} = \frac{3 \times 10^8 \text{ m/s}}{137} = 2.19 \times 10^6 \text{ m/s}$$

 $v_0 = 1$ a.u. is the classical velocity of the electron in the first Bohr's orbit.

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HARTREE ATOMIC UNITS (cont.)





$$t_0 = \frac{a_0}{v_0} = \frac{5.29 \times 10^{-11} \text{m}}{2.19 \times 10^6 \text{ m/s}} = 2.42 \times 10^{-17} \text{s} = 24.2 \text{ as (attoseconds)}$$

How long does a classical electron take to complete the first Bohr's orbit?

$$\frac{\text{space}}{\text{velocity}} = \frac{2\pi a_0}{v_0} = 2\pi \times 2.42 \times 10^{-17} \text{ s} = 152 \text{ as} = 2\pi \text{ a.u.}$$

The atomic unit of frequency is:

$$\frac{1}{t_0} = \frac{v_0}{a_0} = \frac{1}{2.42 \times 10^{-17} \text{s}} = 4.13 \times 10^{16} \text{Hz} \quad (XUV)$$

Excercise 9: (a) How much is the electric field felt by a classical electron in the first Bohr's orbit? V

$$5.14 \times 10^{11} \frac{\text{V}}{\text{m}} = ... = \frac{e}{4\pi\varepsilon_0 a_0^2} = 1 \text{ a.u.}$$

(b) How much is the electric potential felt by a classical electron in the first Bohr's orbit?

27.2 V = ... =
$$\frac{e}{4\pi\varepsilon_0 a_0}$$
 = 1 a.u.

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HARTREE ATOMIC UNITS (cont.)

(c) What is the intensity due to 1 a.u. of electric field?



$$I = \frac{\varepsilon_0 c E_0^2}{2} = \frac{137}{8\pi} = 5.45 \text{ a.u.}$$

$$= \dots = 3.5 \times 10^{16} \frac{\text{W}}{\text{cm}^2}$$

$$\Rightarrow 1 \text{ a.u.} = \frac{3.5 \times 10^{16} \frac{\text{W}}{\text{cm}^2}}{5.45} = 6.44 \times 10^{15} \frac{\text{W}}{\text{cm}^2}$$

The atomic energy of a hydrogen atom in its ground state is:

$$\frac{1}{2}m_{e}v_{0}^{2} - \frac{e^{2}}{4\pi\varepsilon_{0}a_{0}} = \frac{1}{2}m_{e}\frac{\hbar^{2}}{m_{e}^{2}a_{0}^{2}} - \frac{e^{2}}{4\pi\varepsilon_{0}a_{0}} = \frac{1}{2} - 1 = -\frac{1}{2}$$

$$= \dots = -2.18 \times 10^{-18} \text{ J}$$

$$\Rightarrow 1 \text{ a.u.} = 4.36 \times 10^{-18} \text{ J}$$

The atomic unit of momentum is:

$$m_e v_0 = 1 \text{ a.u.}$$

= $9.11 \times 10^{-31} \text{kg} \times 2.19 \times 10^6 \text{ m/s} = 1.99 \times 10^{-24} \text{kg m/s}$

We can derive other physical magnitudes in a.u.