Departamento de Física .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: $m_e = 9.11\times10^{-31}\,\mathrm{kg}$
The atomic unit of charge is the electron charge: $e = 1.602\times10^{-19}\,\mathrm{C}$
The atomic unit of length is the Bohr radius: $a_0 = 5.29\times10^{-11}\,\mathrm{m}$
The atomic unit of angular momentum: $\hbar = \dfrac{h}{2\pi} = 1.05\times10^{-34}\,\mathrm{J.s}$

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

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

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HARTREE ATOMIC UNITS (cont.)

Besides, the angular momentum is: $L = m_e v r = n\hbar \quad \Rightarrow \quad v = \dfrac{n\hbar}{m_e r}$

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

$$a_0 = r_1 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 4\pi\varepsilon_0 = 1 \Rightarrow \varepsilon_0 = \frac{1}{4\pi} = 8.85\times10^{-12}\,\frac{\mathrm{C^2 s^2}}{\mathrm{m^3 kg}}$$

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

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

$$\Rightarrow c = 137.036$$

How much is a speed of 1 a.u.?

$$v_0 = 1 = \frac{c}{137} = \frac{3\times10^8\ \mathrm{m/s}}{137} = 2.19\times10^6\ \mathrm{m/s}$$

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.)

What is the atomic unit of time?

$$t_0 = \frac{a_0}{v_0} = \frac{5.29\times10^{-11}\mathrm{m}}{2.19\times10^6\ \mathrm{m/s}} = 2.42\times10^{-17}\,\mathrm{s} = 24.2 \text{ as (attoseconds)}$$

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

$$\frac{\text{space}}{\text{velocity}} = \frac{2\pi a_0}{v_0} = 2\pi\times2.42\times10^{-17}\,\mathrm{s} = 152 \text{ as} = 2\pi \text{ a.u.}$$

The atomic unit of frequency is:

$$\frac{1}{t_0} = \frac{v_0}{a_0} = \frac{1}{2.42\times10^{-17}\,\mathrm{s}} = 4.13\times10^{16}\,\mathrm{Hz} \quad \text{(XUV)}$$

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

$$5.14\times10^{11}\,\frac{\mathrm{V}}{\mathrm{m}} = \ldots = \frac{e}{4\pi\varepsilon_0 a_0^2} = 1 \text{ a.u.}$$

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

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

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HARTREE ATOMIC UNITS (cont.)

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

$$\left.\begin{aligned} I &= \frac{\varepsilon_0 c E_0^2}{2} = \frac{137}{8\pi} = 5.45 \text{ a.u.} \\ &= \ldots = 3.5\times10^{16}\,\frac{\text{W}}{\text{cm}^2} \end{aligned}\right\} \Rightarrow 1 \text{ a.u.} = \frac{3.5\times10^{16}\,\frac{\text{W}}{\text{cm}^2}}{5.45} = 6.44\times10^{15}\,\frac{\text{W}}{\text{cm}^2}$$

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

$$\tfrac{1}{2} m_e v_0^2 - \frac{e^2}{4\pi\varepsilon_0 a_0} = \tfrac{1}{2} m_e \frac{\hbar^2}{m_e^2 a_0^2} - \frac{e^2}{4\pi\varepsilon_0 a_0} = \tfrac{1}{2} - 1 = -\tfrac{1}{2}$$

$$= \ldots = -2.18\times10^{-18}\,\text{J}$$

$$\Rightarrow 1 \text{ a.u.} = 4.36\times10^{-18}\,\text{J}$$

The atomic unit of momentum is:

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

$$= 9.11\times10^{-31}\,\text{kg}\times2.19\times10^{6}\,\text{m/s} = 1.99\times10^{-24}\,\text{kg m/s}$$

We can derive other physical magnitudes in a.u.