PHYS261 Atomic Physics and Physical Optics

Lecture Wednesday 20. August 2008

Topics:

In lecture: Introduction
Here: Mainly atomic units

Comment:

Introductory Lecture; L. Kocbach

Starting from our page:

http://web.ift.uib.no/AMOS/PHYS261/

History of the Course; Laser Physics; AMOS

Atomic part

Optical part

- We have visited the years of courses – bottom of our page

- We have visited the Atomic units
- The wavelengths – energy and wavenumbers

The Notebook:

- Spectrum of hydrogen,
- Wolfram research (Mathematica) – The world of Physics
- NIST (spectra etc .... National Institute of Standards and Technology)
- Hyperphysics

Atomic Units – the world of Atoms

Wavelengths: the peculiar historical unit of energy

Wavelengths: the peculiar historical unit of energy

Schrödinger Equation (from sometimes ....)

We see that the dimension of energy is kept on both sides

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(r) = E\,\psi(r)$$ is the usual Schrödinger Eq.

$$\nabla^2\psi(r) + k^2\psi(r) = \frac{2m}{\hbar^2}V(r)\,\psi(r) \quad \Big| \quad E\cdot\frac{2m}{\hbar^2} = k^2 \ (\text{for } E>0$$

e^{-r} ? exponential of 3 meters ? $e^{3\,\text{apples}}$?

$e^{-r/\text{length}}$ "All mathematics is dimensionless"

$e^{-\alpha r}$

$[\alpha] = \frac{1}{\text{Length}}$

$[r]$ Length

Atomic units are sometimes "the way to remove dimensions"

$-\frac{\hbar^2}{2m}\nabla^2$ in a.u. $-\frac{1}{2}\nabla^2$

Really: When units well chosen, it is not necessary to write the values of $\hbar$, m, e because they are $\underline{1}$

$V(r) = -\frac{e^2}{r}$ Physics $G(r) = -\varkappa \frac{m_1 M}{r}$

grav. const.

$V(r) = -\frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}$

Unit of charge S.I. e-units
"statcoulomb" chosen historically
"Coulomb"

Atomic units (Gaussian units)

$V(r) = -\frac{e^2}{r}$ e is electron charge

Unit of length is the Bohr radius:

$$a_0 = \frac{\hbar^2}{m_e e^2} \left(= 4\pi\epsilon_0 \frac{\hbar^2}{m_e e^2} \right)$$

The first is in atomic units, second in SI-units. This quantity can be remembered by recalling the virial theorem, i.e. that in absolute value, half of the potential energy is equal to the kinetic energy. This gives us

$$\frac{1}{2}\frac{e^2}{a_0} = \frac{\hbar^2}{2m_e {a_0}^2}$$

and if we accept this relation, we have the above value of a_0.

Unit of length is the Bohr radius:

$$a_0 = \frac{\hbar^2}{m_e e^2} \left(= 4\pi\epsilon_0 \frac{\hbar^2}{m_e e^2} \right)$$

The first is in atomic units, second in SI-units. This quantity can be remembered by recalling the virial theorem, i.e. that in absolute value, half of the potential energy is equal to the kinetic energy. This gives us

$$\frac{1}{2}\frac{e^2}{a_0} = \frac{\hbar^2}{2m_e a_0{}^2}$$

and if we accept this relation, we have the above value of a_0.

$$\frac{\hbar^2}{\cancel{2}m} \cdot \left(\frac{1}{a_0}\right)^2 \quad \text{Kinetic energy "unit"})$$

$$\frac{e^2}{a_0} \qquad \left(-\frac{1}{4\pi\varepsilon_0}\cdots\right) \qquad \frac{e^2}{r}$$

$$\frac{\hbar^2}{m} \cdot \frac{1}{a_0{}^2} = \frac{e^2}{a_0} \qquad E_{au} = \frac{e^2}{\frac{\hbar^2}{me^2}}$$

$$0.529\ \text{Å} \qquad \boxed{a_0 = \frac{\hbar^2}{me^2}} \qquad \rightarrow \frac{me^4}{\hbar^2}$$

$$\boxed{E_{au} = 27.2\,eV}$$

TIME

$$\text{time a.u.} = \frac{\hbar}{\text{Energy a.u.}} \quad (\approx 10^{-17}\ \text{sec})$$