ATOMIC UNITS AND MEASURES OF INTENSITY

Atomic units greatly simplify the appearance of expressions in atomic physics, and these units are thus widely used. They are due to Hartree. The basic atomic units are summarized, and then various measures of electromagnetic field quantities are introduced in terms of atomic units, and relations among these field quantities are summarized.

I.1 ATOMIC UNITS

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Atomic units are specified by the requirement that

$$\hbar = 1, \qquad m = 1, \qquad e^2 = 1, \tag{I.1}$$

where m and e^2 refer, respectively, to the mass of the electron and the squared charge of the electron. These units then are applied in terms of the properties of the simple hydrogen atom based on infinite mass of the atomic nucleus. A single atomic unit of the most important physical quantities is then:

Unit of length: Bohr radius = $a_0 = \hbar^2/\left(me^2\right) \equiv 1$ a.u. = $5.29177249 \times 10^{-11}$ m. Unit of velocity: Velocity of an electron in the first Bohr orbit = $v_0 = e^2/\hbar \equiv 1$ a.u. = 2.18769142×10^6 m/s.

Unit of time: Time for an electron to travel a distance a_0 at the velocity $v_0 = \tau_0 = a_0/v_0 = \hbar^3/me^4 \equiv 1 \text{ a.u.} = 2.41888433 \times 10^{-17} \text{ s.}$

Unit of frequency: Inverse of the unit of time = $\nu_0 = 1/\tau_0 = me^4/\hbar^3 \equiv 1$ a.u. = $4.13413732 \times 10^{16}$ Hz.

Unit of energy: Twice the binding energy of hydrogen $= E_0 = 2R_{\infty} = me^4/\hbar^2 = 1 \text{ a.u.} = 27.2113962 \text{ eV}.$

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I.2 ELECTROMAGNETIC FIELD QUANTITIES

I.2.1 Basic Field Quantities

Unit of electric field strength: $E_0 = E_0/a_0 = m^2 e^5/\hbar^4 \equiv 1 \text{ a.u.} = 5.14220826 \times 10^{11} \text{ V/m}.$

Unit of energy flux (intensity): $I_0 = cE_0^2/(8\pi) = 3.50944758 \times 10^{16} \,\text{W/cm}^2$.

I.2.2 Convenient Relations

Angular frequency in a.u. and wavelength in nm: $\omega(a.u.) = 45.5633526/\lambda(nm)$. Velocity of light and the fine structure constant: $c = 1/\alpha$.

I.2.3 Field Measures Useful in Strong-Field Atomic Physics

To set the convention used for the amplitudes, we shall regard a monochromatic linearly polarized field as being of the form

$$\mathbf{E} = E_0 \epsilon \sin(\omega t - \mathbf{k} \cdot \mathbf{r}), \qquad \epsilon \cdot \epsilon = 1; \tag{I.2}$$

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and a circularly polarized monochromatic field as being of the form

$$\mathbf{E} = \frac{E_0}{2^{1/2}} \left[\mathbf{e}_x \sin(\omega t - \mathbf{k} \cdot \mathbf{r}) \pm \mathbf{e}_y \cos(\omega t - \mathbf{k} \cdot \mathbf{r}) \right], \tag{I.3}$$

$$\mathbf{e}_x \cdot \mathbf{e}_x = \mathbf{e}_y \cdot \mathbf{e}_y = 1, \qquad \mathbf{e}_x \cdot \mathbf{e}_y = 0.$$

In Eq. (I.3), the presumption is that wave propagation is along the z axis, and \mathbf{e}_x , \mathbf{e}_y are unit vectors along the x and y axes, respectively. Whereas the use of the amplitude E_0 in Eq. (I.2) is universal, the definition employed in Eq. (I.3) is not. Some authors omit the factor $2^{-1/2}$. Equations (I.2) and (I.3) have the amplitude relations

$$|\mathbf{E}| = \begin{cases} E_0, & \text{linear} \\ E_0/2^{1/2}, & \text{circular} \end{cases},$$

$$\langle \mathbf{E}^2 \rangle = \begin{cases} \frac{1}{2} |\mathbf{E}|^2 = \frac{1}{2} E_0^2, & \text{linear} \\ |\mathbf{E}|^2 = \frac{1}{2} E_0^2, & \text{circular} \end{cases},$$
(I.4)

where the angle bracket indicates a time average over a period.

Irradiance, or Energy Flux

A physical quantity frequently employed to measure the "strength" of the field is often expressed in units of Watts/cm², or Joules/($s \cdot cm^2$). This is a flux of energy, also known as irradiance. It has, however, now become quite common to refer to this

quantity simply as the intensity. We shall here use the designation *I* for the irradiance, given by the amplitude of the Poynting vector, or

I (Gaussian units) =
$$uc = \frac{c}{4\pi} \langle \mathbf{E}^2 \rangle = \frac{c}{8\pi} E_0^2$$
.

The atomic unit of irradiance I_0 , as indicated above, is that energy flux that corresponds to $E_0 = 1$ a.u., so that $I_0 = c/(8\pi) = 3.50944758 \times 10^{16} \,\text{W/cm}^2$.

When all quantities are in atomic units, then

$$I=2\left\langle \mathbf{E}^{2}\right\rangle =E_{0}^{2}.$$

Ponderomotive Energy

The ponderomotive energy is that energy that a free charged particle possesses because of its oscillation, or "quiver," motion when in an electromagnetic field. It is exactly the kinetic energy of such oscillatory motion as expressed in the frame of reference in which the center of mass (c.m.) of the charged particle is, on a time average, at rest. If a charged particle should emerge adiabatically from a region in which there is an electromagnetic field into a region free of the field, this ponderomotive energy is converted into a directed kinetic energy. The ponderomotive energy U_p is thus sometimes called the ponderomotive potential. In atomic units,

$$U_p = \frac{I}{4\omega^2} = \frac{\langle \mathbf{E}^2 \rangle}{2\omega^2} = \left(\frac{E_0}{2\omega}\right)^2.$$

Free-Electron Amplitude of Motion

The amplitude of motion of an electron in a plane wave field is often designated α_0 . As expressed in the frame of reference in which the c.m. of the electron is at rest on the average, this motion is a rectilinear oscillation along the polarization direction for a linearly polarized plane wave of moderate intensity, with

$$\alpha_0 = \frac{I^{1/2}}{\omega^2} = \frac{2}{\omega} U_p^{1/2} = \frac{E_0}{\omega^2}.$$

This result is actually the limit of the true relativistic motion of the electron, where the relativistic nature of the motion will arise as a result of the intensity of the field. The relativistic motion is in the form of a figure 8, with the axis of the lobes along the polarization direction, and the plane of the figure 8 determined by the polarization direction and the direction of propagation.

For a circularly polarized electromagnetic field, the electron motion in the simplest frame of reference is a circle executed in the plane perpendicular to the direction of propagation. This circle has the radius

$$\alpha_0 = \frac{1}{\omega^2} \left(\frac{I}{2} \right)^{1/2} = \frac{(2U_p)^{1/2}}{\omega} = \frac{E_0}{2^{1/2} \omega^2}.$$

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The Keldysh parameter, or adiabaticity parameter, is actually an inverse intensity parameter. It is given as

$$\gamma = \frac{\omega (2E_i)^{1/2}}{E_0} = \frac{\omega (2E_i)^{1/2}}{I^{1/2}} = \frac{E_i^{1/2}}{(2U_p)^{1/2}},$$

where E_i is the ionization potential of the atom.

The inverse square of the adiabaticity parameter is directly an intensity parameter, which can be defined *ab initio* as twice the ratio of the ponderomotive energy to the ionization potential of the atom. When used in this form, it is generally designated z_1 , where

$$z_1 \equiv \frac{2U_p}{E_i} = \frac{I}{2\omega^2 E_i} = \frac{E_0^2}{2\omega^2 E_i} = \begin{cases} (\omega \alpha_0)^2 / (2E_i), & \text{linear} \\ (\omega \alpha_0)^2 / E_i, & \text{circular} \end{cases}$$

This quantity has been called the bound-state intensity parameter.

Another intensity parameter is the ratio of the ponderomotive energy of the electron to the energy of a single photon of the field. That is, it is given by

$$z \equiv \frac{U_p}{\omega} = \frac{I}{4\omega^3} = \frac{E_0^2}{4\omega^3} = \begin{cases} \omega \alpha_0^2 / 4, & \text{linear} \\ \omega \alpha_0^2 / 2, & \text{circular} \end{cases}$$
.

This quantity has been called the *intensity parameter for the final continuum state*, and also the *nonperturbative intensity parameter*, since it is the quantity that is the primary indicator of when perturbation theory will fail.

There is a free-electron parameter that always arises in the description of the interaction of a free electron with an electromagnetic field. There is no universally accepted symbol for this parameter, although many authors have defined the very same quantity. We here designate it z_f . It is most readily defined as twice the ratio of the ponderomotive energy of the electron in the field to the rest energy of the electron, or

$$z_f \equiv \frac{2U_p}{c^2} = \frac{I}{2(\omega c)^2} = \frac{1}{2} \left(\frac{E_0}{\omega c}\right)^2 = \begin{cases} \frac{1}{2}(\omega \alpha_0/c)^2, & \text{linear} \\ (\omega \alpha_0/c)^2, & \text{circular} \end{cases}$$

By its definition, this parameter plainly is a measure of the appearance of relativistic effects in the field-induced motion of an electron. It is the *free-electron intensity* parameter.