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Units and Constants

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1.1 PHYSICAL CONSTANTS

The currently accepted values for the physical constants are listed in Table 1.1, based on the 1986 CODATA(Committee on Data for Science and Technology) recommendations [1]. Although improved measurements are now available for several of the entries [2], they cannot readily be incorporated with the 1986 values until the next complete least-squares adjustment of the constants. The recommended values therefore remain as tabulated. The one exception is the value of the Rydberg constant R_∞, which has been updated to reflect the fifty-fold improvement in its measurement in units of m^{-1} (or equivalently in units of Hz, since the conversion factor c is a defined physical constant) [3]. Because the uncertainties are correlated, the full variance matrix must be used in calculating uncertainties for further quantities in terms of those tabulated.

1.2 ELECTROMAGNETIC UNITS

The standard electromagnetic units adopted by most scientific journals and elementary texts belong to the *système international* (SI) or rationalized MKSA (meters, kilograms, seconds, and amperes) units. However, many authors working with microscopic phenomena prefer *Gaussian* units, and theoretical physicists often use *Heaviside-Lorentz* (H-L) units. In this Handbook, SI units are used together with *atomic units.* The current section is meant as a reference relating these different systems.

The relations among different sets of units are not simple conversions since the same symbol in different systems can have different physical dimensions. To clarify the meanings of the units, we summarize basic electromagnetic relations for SI, Gaussian, and H-L systems below. The Coulomb law for the magnitude F of the force acting on each of two static charges q and Q separated by a distance r in a homogeneous medium of permittivity ϵ can be written

$$F = \frac{1}{4\pi\epsilon}\frac{qQ}{r^2}\,, \tag{1.1}$$

where in a vacuum, ϵ is[1]

$$\epsilon_0 = \begin{cases} \left(\mu_0 c^2\right)^{-1}, & \text{SI} \\ (4\pi)^{-1}, & \text{Gaussian} \\ 1, & \text{H-L}\,, \end{cases} \tag{1.2}$$

with the closely related permeability of vacuum given by

$$\mu_0 = \begin{cases} 4\pi\times 10^{-7}\,\mathrm{N/A^2}, & \text{SI} \\ 4\pi\,, & \text{Gaussian} \\ 1, & \text{H-L}\,. \end{cases} \tag{1.3}$$

[1] We deviate here from Jackson [4] who takes $\epsilon_0 = \mu_0 = 1$ in Gaussian units and must introduce additional constants to relate the units. The physically important quantities are the *relative values* $\epsilon_r \equiv \epsilon/\epsilon_0$ and $\mu_r \equiv \mu/\mu_0$, which in traditional Gaussian-unit notation are written without the r subscript.

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Table 1.1. Table of physical constants. Uncertainties are given in parentheses.

Quantity	Symbol	Value	Units
speed of light in vacuum	c	2.997 924 58	10^8 m s^{-1}
gravitational constant	G	6.672 59(85)	10^{-11} m^{3}kg^{-1}m^{-2}
Planck constant	h	6.626 075 5(40)	10^{-34} J s
	$\hbar = h/2\pi$	1.054 572 66(63)	10^{-34} J s
elementary charge	e	1.602 177 33(49)	10^{-19} C
		4.803 206 8(15)	10^{-10} esu
inverse fine structure constant, $4\pi\epsilon_0\hbar c/e^2$	α^{-1}	137.035 989 5(61)	
magnetic flux quantum, $h/2e$	Φ_0	2.067 834 61(61)	10^{-15} Wb
atomic mass unit, $\frac{1}{12}m(^{12}\mathrm{C})$	$m_\mathrm{u} = u$	1.660 540 2(10)	10^{-27} kg
	$m_\mathrm{u}c^2$	931.494 32(28)	MeV
electron mass	m_e	9.109 389 7(54)	10^{-31} kg
		5.485 799 03(13)	10^{-4} u
muon mass	m_μ	0.113 428 913(17)	u
proton mass	m_p	1.007 276 470(12)	u
neutron mass	m_n	1.008 664 904(14)	u
deuteron mass	m_d	2.013 553 214(24)	u
α-particle mass	m_α	4.001 506 178(84)	u
Rydberg constant, $m_\mathrm{e}c\alpha^2/2h$	R_∞	1.097 373 156 834(24)	10^7 m^{-1}
	$R_\infty c$	3.289 841 960 305(72)	10^{15} Hz
	$R_\infty hc$	13.605 698 1(40)	eV
		2.179 874 1(13)	10^{-18} J
Bohr radius, $\alpha/4\pi R_\infty$	a_0	0.529 177 249(24)	10^{-10} m
Hartree energy, $e^2/[4\pi\epsilon_0]a_0 = 2R_\infty hc$	E_h	27.211 396 1(81)	eV
	E_h/h	6.579 683 920 61(14)	10^{15}Hz
	E_h/hc	2.194 746 313 668(48)	10^7 m^{-1}
Compton wavelength, αa_0	$\lambda\!\!\!^{-}_\mathrm{C} = \lambda_\mathrm{C}/2\pi$	3.861 593 23(35)	10^{-13} m
classical electron radius, $\alpha^2 a_0$	r_e	2.817 940 92(38)	10^{-15} m
Thomson cross section, $8\pi r_\mathrm{e}^2/3$	σ_e	0.665 246 16(18)	10^{-28} m^2
Bohr magneton, $e\hbar/2m_\mathrm{e}$	μ_B	9.274 015 4(31)	10^{-24} J T^{-1}
		5.788 382 63(52)	10^{-5} eV T^{-1}
electron magnetic moment	$\mu_\mathrm{e}/\mu_\mathrm{B}$	1.001 159 652 193(10)	
muon magnetic moment	μ_μ/μ_B	4.841 970 97(71)	10^{-3}
proton magnetic moment	$\mu_\mathrm{p}/\mu_\mathrm{B}$	1.521 032 202(15)	10^{-3}
neutron magnetic moment	$\mu_\mathrm{n}/\mu_\mathrm{B}$	1.041 875 63(25)	10^{-3}
deuteron magnetic moment	$\mu_\mathrm{d}/\mu_\mathrm{B}$	0.466 975 447(91)	10^{-3}
electron g factor $2(1+a_\mathrm{e})$	g_μ	2.002 319 304 386(20)	
muon g factor $2(1+a_\mu)$	g_μ	2.002 331 846(17)	
proton gyromagnetic ratio	γ_p	2.675 221 28(81)	10^8 s^{-1}T^{-1}
Avogadro constant	N_A	6.022 136 7(36)	10^{23} mol^{-1}
Faraday constant, $N_\mathrm{A}e$	F	9.648 530 9(29)	10^4 C mol^{-1}
Boltzmann constant	k_B	1.380 658(12)	10^{-23} J K^{-1}
		8.617 385(73)	10^{-5} eV K^{-1}
	$k_\mathrm{B}/E_\mathrm{h}$	3.166 830(27)	10^{-6} K^{-1}
molar gas constant	R	8.314 510(70)	J mol^{-1} K^{-1}
molar volume (ideal gas), RT/P			
$T = 273.15$ K, $P = 101.325$ kPa	V_m	0.022 414 10(19)	m^3 mol^{-1}
$T = 273.15$ K, $P = 100$ kPa	V_m	0.022 711 08(19)	m^3 mol^{-1}
Stefan-Boltzmann constant $\pi^2 k_\mathrm{B}^4/(60\hbar^3c^2)$	σ	5.670 51(19)	10^{-8} W m^{-2} K^{-4}
first radiation constant, $2\pi hc^2$	c_1	3.741 774 9(22)	10^{-16} W m^2
second radiation constant, hc/k_B	c_2	0.014 387 69(12)	m K
Wien displacement constant, $\lambda_{\max}T = c_2/4.965\,114\,23$	b	2.897 756(24)	10^{-3} m K

Note that ϵ_0 and μ_0 are dimensionless in H-L and Gaussian units, but not in the SI units. Current or electric charge is an independent quantity in the MKSA system but can be expressed in purely mechanical dimensions in the H-L and Gaussian systems. Thus, in Gaussian units, 1 statcoulomb = 1 dyne$^{1/2}$cm, but in SI, even though the ampere is *defined* in terms of the attractive force between thin parallel wires carrying equal currents, there is no mechanical equivalent for the ampere or the coulomb. To establish such an equivalence, one can supplement the SI units by assigning a dimensionless number to ϵ_0 or to μ_0. Gaussian and H-L units arise from two different assignments. The result of assigning a number to ϵ_0 is analogous to the relation 1 s = $\dot{3} \times 10^8$ m established between time and distance units if one sets the speed of light $c = 1$, a convention often used in conjunction with H-L units. (Note that for simplicity, the pure number 2.997 924 58, equal numerically to the defined speed of light in vacuum in units of 10^8 m/s, is represented by $\dot{3}$.) Thus, although within the Gaussian system, where the assignment $4\pi\epsilon_0 = 1$ is made, it is justified to assert that 1 coulomb *equals* $\dot{3} \times 10^9$ statcoulombs, this is not true in pure SI, where there is no equivalent mechanical unit for charge.

Maxwell's macroscopic equations can be written

$$\begin{aligned} \lambda\nabla\cdot\mathbf{D} &= \rho\,, \\ \lambda c'\nabla\times\mathbf{H} - \lambda\frac{\partial\mathbf{D}}{\partial t} &= \mathbf{j}\,, \\ c'\nabla\times\mathbf{E} + \frac{\partial\mathbf{B}}{\partial t} &= 0\,, \\ \nabla\cdot\mathbf{B} &= 0\,, \end{aligned} \tag{1.4}$$

with the macroscopic field variables related to the polarizations $\mathbf{P}$ and $\mathbf{M}$ by

$$\begin{aligned} \lambda\mathbf{D} &= \epsilon_0\mathbf{E} + \mathbf{P} = \epsilon\mathbf{E} \\ \lambda\mathbf{H} &= \mu_0^{-1}\mathbf{B} - \mathbf{M} = \mathbf{B}/\mu \end{aligned} \tag{1.5}$$

(the last equalities for $\mathbf{D}$ and $\mathbf{H}$ hold only for homogeneous media) and

$$\lambda = \begin{cases} 1, & \text{SI} \\ \epsilon_0 = \mu_0^{-1}, & \text{Gaussian or H-L}\,, \end{cases} \tag{1.6}$$

$$c' = \begin{cases} 1, & \text{SI} \\ c, & \text{Gaussian or H-L}\,. \end{cases} \tag{1.7}$$

In Gaussian or H-L units, fields $\mathbf{E}, \mathbf{B}, \mathbf{D}, \mathbf{H}$, and polarizations (dipole moments per unit volume) $\mathbf{P}, \mathbf{M}$ all have the same dimensions, whereas in SI units the microscopic fields $\mathbf{E}$ and $\mathbf{B}$ have dimensions that are generally distinct from each other as well as from $\mathbf{P}$ (or $\mathbf{D}$) and $\mathbf{M}$ (or $\mathbf{H}$) respectively. In all three unit systems, the dimensionless ratio ϵ/ϵ_0 is called the dielectric constant (or relative permittivity) of the medium, and the (dimensionless) fine-structure constant is

$$\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \tag{1.8}$$

with a numerical value $\alpha^{-1} = 137.035\,989\,5\,(61)$.

In atomic units (see Sect. 1.3), the factor $e^2/(4\pi\epsilon_0)$, the electron mass m_e, and $\hbar$, Planck's constant divided by 2π, are all equal to 1. In Gaussian and H-L systems, these conditions determine a numerical value for all electromechanical units. Thus in Gaussian units, the electronic charge is $e = 1$ whereas in H-L units $e = \sqrt{4\pi}$. In the SI system, on the other hand, the three conditions $e^2/(4\pi\epsilon_0) = m_e = \hbar = 1$ determine numerical values for mechanical units but not for electromagnetic ones. A complete determination of values requires that ϵ_0 also be assigned a value. The choice most consistent with previous work is to take $e = 1 = 4\pi\epsilon_0$. This choice is made here.

Since a volt is a joule/coulomb and a statvolt is an erg/statcoulomb, 1 volt corresponds to (but is not generally *equal* to, since the physical dimensions may differ)

$$\frac{10^7\,\text{erg}}{2\,997\,924\,580\,\text{statcoulomb}} = \frac{1}{\dot{3}00}\,\text{statvolt}\,. \tag{1.9}$$

In Gaussian units, the unit of magnetic field, namely Gauss ($\mathbf{B}$) or Oersted ($\mathbf{H}$) has the same physical size and dimension as the unit of electric field, namely statvolt/cm, which in turn corresponds to an SI field of $\dot{3} \times 10^4$ V/m. However, the tesla (1 T = 1 weber/m^2), the SI unit of magnetic field $\mathbf{B}$ (older texts refer to $\mathbf{B}$ as the *magnetic induction*), has the physical dimensions of V s/m^2. To find the correspondence to Gaussian units, one must multiply by the speed of light c:

$$1\,\text{T}\,c = \dot{3} \times 10^8\,\text{V/m} \tag{1.10}$$

which corresponds to 10^4 statvolt/cm and hence to 10^4 gauss.

Below are two tables relating basic mechanical and electromagnetic quantities. Caution is required both because the same symbol often stands for quantities of different physical dimensions in different systems of units, and because factors of 2π sometimes enter frequencies, depending on whether the units are cycles/s (Hz) or radians/s. The double-headed arrows ($\leftrightarrow$) indicate a correspondence between quantities whose dimensions are not necessarily equal. Thus for example, the force on an electron due to a Gaussian electric field of 1 statvolt/cm is the same as due to an SI electric field of $\dot{3} \times 10^4$ V/m. The correspondences between Gaussian and SI electrostatic quantities become equalities if and only if $4\pi\epsilon_0 = 1$. Thus they are equalities within the Gaussian system but not within the less constrained SI scheme. The SI and Gaussian units of magnetic field have different dimensions unless both ϵ_0 and c are set equal to dimensionless numbers. *Natural H-L*

Table 1.2. Conversion factors for various physical quantities.

Quantity	SI units	Gaussian units	Natural H-L units: $\hbar = c = \epsilon_0 = 1$
length	1 m	$= 10^2$ cm	$= 1$ m
mass	1 kg	$= 10^3$ g	$\leftrightarrow 3.519\,341\,3\,(21) \times 10^8$ m^{-1}
time	1 s	$= 1$ s	$\leftrightarrow 2.997\,924\,58 \times 10^8$ m
velocity	1 m/s	$= 10^2$ cm/s	$\leftrightarrow 3.335\,640\,951\,98 \cdots \times 10^{-9}$
energy	1 J=1 kg m^2/s^2	$= 10^7$ erg	$\leftrightarrow 3.163\,026\,2\,(19) \times 10^{25}$ m^{-1}
action	1 J s	$= 10^7$ erg s	$\leftrightarrow 0.948\,251\,40\,(57) \times 10^{34}$
force	1 N = 1 J/m	$= 10^5$ dyne	$\leftrightarrow 3.163\,026\,2\,(19) \times 10^{25}$ m^{-2}
power	1 W = 1 J/s	$= 10^7$ erg/s	$\leftrightarrow 1.055\,071\,97\,(63) \times 10^{33}$ m^{-2}
intensity	1 W/m^2	$= 10^3$ erg/cm^2	$\leftrightarrow 1.055\,071\,97\,(63) \times 10^{33}$ m^{-2}
charge	1 C = 1 A s	$\leftrightarrow \dot{3} \times 10^9$ statcoul	$\leftrightarrow 1.993\,684\,01\,(61) \times 10^{13}$
potential	1 V = 1 J/C	$\leftrightarrow 1/\dot{3}00$ statvolt	$\leftrightarrow 1.586\,523\,3\,(11) \times 10^{12}$ m^{-1}
electric field	1 V/m = 1 N/C	$\leftrightarrow \left(\dot{3} \times 10^4\right)^{-1}$ statvolt/cm	$\leftrightarrow 1.586\,523\,3\,(11) \times 10^{12}$ m^{-2}
magnetic field	1 T = 1 N/(A m)	$\leftrightarrow 10^4$ gauss	$\leftrightarrow 4.756\,277\,3\,(32) \times 10^{20}$ m^{-2}

Table 1.3. Physical quantities in atomic units with $\hbar = e = m_e = 4\pi\epsilon_0 = 1$, and $\alpha^{-1} = 137.035\,989\,5\,(61)$.

Quantity	Unit	Value
length	a_0	$0.529\,177\,249\,(24) \times 10^{-10}$ m
mass	m_e	$0.910\,938\,97\,(54) \times 10^{-30}$ kg
time	$\hbar/E_h$	$2.418\,884\,326\,555\,(53) \times 10^{-17}$ s
velocity	$v_B \equiv \alpha c$	$2.187\,691\,42(10) \times 10^6$ m/s
energy	E_h	$4.359\,748\,2(26) \times 10^{-18}$ J
action	$\hbar$	$1.054\,572\,66\,(63) \times 10^{-34}$ J s
force	E_h/a_0	$0.823\,872\,95\,(49) \times 10^{-7}$ N
power	$E_h^2/\hbar$	$0.180\,237\,98\,(11)$ W
intensity	$\dfrac{E_h^2}{\hbar a_0^2}$	$64.364\,142\,(39) \times 10^{18}$W/m^2
charge	e	$1.602\,177\,33\,(49) \times 10^{-19}$ C
potential	E_h/e	$27.211\,396\,1\,(81)$ V
electric field	$\dfrac{E_h}{ea_0}$	$0.514\,220\,82\,(15) \times 10^{12}$ V/m
magnetic field	$\dfrac{E_h}{ea_0\alpha c}$	$2.350\,518\,09\,(71) \times 10^5$ tesla

units can be considered SI units supplemented by the conditions $\epsilon_0 = c = \hbar = 1$. They are listed here in units of meters, although eV are also often used: 1 eV = $5.067\,728\,9\,(15) \times 10^6$ m$^{-1} \times \hbar c$. The correspondences may be considered equalities within the natural H-L system but not within SI. More electromagnetic conversions can be found in Jackson [4]. The data here are based mainly on the 1986 adjustment by Cohen and Taylor [1] with the 1993 correction to the Rydberg constant[3].

A few additional energy conversion factors are

$$
\begin{aligned}
1\text{ eV} &= 1.602\,177\,33\,(49) \times 10^{-19}\text{ J} \\
&= 2.417\,988\,36\,(72) \times 10^{14}\text{ Hz} \times h \\
&= 8\,065.541\,0(24)\ \text{cm}^{-1} \times hc \\
&= 3.674\,930\,9\,(11) \times 10^{-2}\ E_h \\
&= 1.106\,044\,5\,(10) \times 10^4\text{ K} \times k_B \\
&= 23.049\,524\,(20)\ \text{kcal/mol} \\
&= 96.485\,309\,(82)\ \text{kJ/mol}
\end{aligned}
$$

The basic unit of temperature, the kelvin, is equivalent to about 0.7 cm^{-1}, i.e., the value of the Boltzmann constant k_B expressed in wavenumber units per kelvin is $0.695\,039(6)$ cm^{-1}/K. Since K is the internationally accepted symbol for the kelvin [5], this suggests that the use of the letter K as a symbol for 1 cm^{-1} (1 kayser) should be discontinued.

1.3 ATOMIC UNITS

Atomic and molecular calculations based on the Schrödinger equation are most conveniently done in atomic units (a.u.), and then the final result converted to the correct SI units as listed in Table 1.3. In atomic units, $\hbar = m_e = e = 4\pi\epsilon_0 = 1$. The atomic units of length, velocity, time, and energy are then

$$
\begin{aligned}
\text{length}: \quad & a_0 = \frac{\hbar^2}{m_e e^2} = \frac{\hbar}{\alpha m_e c}, \\
\text{velocity}: \quad & v_B = e^2/\hbar = \alpha c, \\
\text{time}: \quad & \tau_0 = \frac{\hbar^3}{m_e e^4} = \frac{\hbar}{\alpha^2 m_e c^2}, \\
\text{energy}: \quad & E_h = e^2/a_0 = \alpha^2 m_e c^2,
\end{aligned}
$$

where, from the definition (1.8), the numerical value of c is $\alpha^{-1} = 137.035\,9895(61)$ a.u. For the lowest $1s$ state of hydrogen (with infinite nuclear mass), a_0 is the Bohr radius, v_B is the Bohr velocity, $2\pi\tau_0$ is the time to complete a Bohr orbit, and E_h (the Hartree energy) is twice the ionization energy. To include finite nuclear mass effects, replace m_e by the electron reduced mass $\mu = M/(M + m_e)$.

Atomic energies are often expressed in units of the Rydberg (Ry). The Rydberg for an atom having nuclear mass M is

$$1 \text{ Ry} = R_M = M(M + m_e)^{-1} R_\infty , \tag{1.11}$$

with

$$R_\infty = m_e c\alpha^2/(2h) = 10\,973\,731.568\,3(3) \text{ m}^{-1} \tag{1.12}$$

which is equivalent to 13.605 698(4) eV. The Rydberg constant R_∞ is thus the limit value for infinite nuclear mass.

The energy equivalent of the electron mass, $m_e c^2$, is 510.999 06(15) keV. This energy is a natural unit for relativistic atomic theory. For example, for inner-shell energies in the heaviest elements, the binding energy of the 1s electron in hydrogenic Lr (Z=103) is 0.338 42 $m_e c^2$.

1.4 MATHEMATICAL CONSTANTS

A selection of the most important mathematical constants is listed in Table 1.4. More extensive tabulations and formulas can be found in the standard mathematical works [6, 7] (see also Chap. 9).

1.4.1 Series Summation Formula

The Riemann zeta function defined by $\zeta(n) = \sum_{i=1}^{\infty} i^{-n}$ (see Table 1.4) is particularly useful in summing slowly convergent series of the form

$$S = \sum_{i=1}^{\infty} T_i \,. \tag{1.13}$$

For example, suppose that the series

$$T_i = t_2 i^{-2} + t_3 i^{-3} + \cdots \tag{1.14}$$

for the individual terms in S is rapidly convergent for $i > N$, where N is some suitably large integer. Then

$$S = \sum_{i=1}^{N} T_i + t_2 \zeta^N(2) + t_3 \zeta^N(3) + \cdots , \tag{1.15}$$

where $\zeta^N(n) = \zeta(n) - \sum_{i=1}^{N} i^{-n}$ is the zeta function with the first N terms subtracted. For N sufficiently large, only the first few t_j coefficients need be known, and they can be adequately estimated by solving the system of equations

Table 1.4. Values of e, π, Euler's constant γ, and the Riemann zeta function $\zeta(n)$.

Constant	Value
e	2.718 281 828 459 045 235 360 287 471 352 66
π	3.141 592 653 589 793 238 462 643 383 279 50
$\pi^{1/2}$	1.772 453 850 905 516 027 298 167 483 341 14
γ	0.577 215 664 901 532 860 606 512 090 082 40
$\zeta(2)$	1.644 934 066 848 226 436 472 415 166 646 02
$\zeta(3)$	1.202 056 903 159 594 285 399 738 161 511 45
$\zeta(4)$	1.082 323 233 711 138 191 516 003 696 541 16
$\zeta(5)$	1.036 927 755 143 369 926 331 365 486 457 03
$\zeta(6)$	1.017 343 061 984 449 139 714 517 929 790 92
$\zeta(7)$	1.008 349 277 381 922 826 839 797 549 849 80
$\zeta(8)$	1.004 077 356 197 944 339 378 685 238 508 65
$\zeta(9)$	1.002 008 392 826 082 214 417 852 769 232 41
$\zeta(10)$	1.000 994 575 127 818 085 337 145 958 900 31

$$T_N = t_2 N^{-2} + t_3 N^{-3} + \cdots + t_{k+2} N^{-k-2} , \tag{1.16a}$$

$$T_{N-1} = t_2(N-1)^{-2} + t_3(N-1)^{-3} + \cdots + t_{k+2}(N-1)^{-k-2} , \tag{1.16b}$$

$$\vdots$$

$$T_{N-k} = t_2(N-k)^{-2} + t_3(N-k)^{-3} + \cdots + t_{k+2}(N-k)^{-k-2} , \tag{1.16c}$$

where $k + 1 \le N$ is the number of terms retained in Eq. (1.14).

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