THERMO_PW

Units guide (v.1.6.0)

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Chapter 1

Introduction

These notes discuss the atomic units (a.u.) used in electronic structure codes. They are updated with the recent (year 2019) changes to the international system (SI). The conversion factors written here should be those implemented in the QUANTUM ESPRESSO and `thermo_pw` codes.
These notes are part of the `thermo_pw` package. The complete package is available at `https://github.com/dalcorso/thermo_pw`.

1.1 People

These notes have been written by Andrea Dal Corso (SISSA - Trieste).
Disclaimer: I am not an expert of units. These notes reflect what I think about units. If you think that some formula is wrong, that I misunderstood something, or that something can be calculated more simply, please let me know, I would like to learn more. You can contact me by e-mail: `dalcorso@sissa.it`.

1.2 Overview

Electronic structure codes use atomic units (a.u.). In these notes we explain how to obtain the conversion factors from a.u. to the international system (SI) units and viceversa. The most relevant physical formulas are written both in SI units and in a.u.. Moreover, since several books and old literature still use the c.g.s. (centimeter-gram-second) system we discuss also how to convert from a.u. to c.g.s.-Gaussian units and viceversa.

These notes are organized in Sections, one for each physical quantity. For each quantity we give its definition in the SI system and then we derive the conversion factor from the a.u. to the SI unit, the conversion factor from the c.g.s-Gaussian unit to the SI unit, and the conversion factor from the a.u. to the c.g.s-Gaussian unit. The text in each Section depends on the definitions given in previous Sections. Only in a few cases it depends on definitions given in following Sections and in these cases we mention explicitly where to find the required definition. Important physical formulas are introduced when we have given sufficient information to convert the formula in different systems. Microscopic and macroscopic Maxwell's equations are also summarized in separate Sections.
Each system has a different color. In black the SI, in blue the a.u., in orange the c.g.s.-Gaussian system, and in green the conversion factors from a.u. to the c.g.s.-Gaussian units. Comments of interest not belonging to any system in particular are given in red. We indicate the numerical value of a given quantity in the SI with a tilde. The units in a.u. are indicated with a bar, while the units in the c.g.s.-Gaussian system are indicated with a bar and the subscript cgs. When the c.g.s.-Gaussian unit has an accepted name we use it interchangeably with the generic name. Only Hartree a.u. are described in the main text since these are the most common microscopic units. QUANTUM ESPRESSO uses Rydberg a.u. that can be easily derived from the Hartree a.u.. We describe Rydberg a.u. in Appendix A (in purple). In the $ab-initio$ literature modified a.u. have been introduced in which the electromagnetic equations look like those of the c.g.s-Gaussian system. This requires some modifications to the definitions given in the main text and we discuss these units in Appendix B (in steelblue).

It is useful to recall a few preliminary facts needed in the rest of these notes. A few experimental quantities have fixed values in the SI. Among these:
The Planck constant

$$h = 6.62607015 \times 10^{-34} \ \mathrm{J \cdot s}, \tag{1.1}$$

the speed of light

$$c = 2.99792458 \times 10^{8} \ \mathrm{m/s}, \tag{1.2}$$

and the electron charge

$$e = 1.602176634 \times 10^{-19} \ \mathrm{C}. \tag{1.3}$$

Two experimental quantities are known with high accuracy:
The Rydberg constant, measured spectroscopically from the frequencies of

Hydrogen and Deuterium absorption and emission lines:

$$R_\infty = 1.0973731568160 \times 10^7\ 1/\mathrm{m} \tag{1.4}$$

is known with a relative error of 1.9×10^{-12}
and the fine structure constant, measured from the anomaly of the electron magnetic moment,

$$\alpha = 7.2973525693 \times 10^{-3}, \tag{1.5}$$

is known with a relative error of 1.6×10^{-10}.

The Rydberg constant can be written in terms of the fine structure constant α and the electron mass m_e or in terms of α and of the Bohr radius a_B:

$$R_\infty = \frac{\alpha^2 m_e c}{2h} = \frac{\alpha}{4\pi a_B}. \tag{1.6}$$

Using these equations we can calculate the electron mass as:

$$m_e = \frac{2hR_\infty}{\alpha^2 c} = 9.1093837015 \times 10^{-31}\ \mathrm{kg} \tag{1.7}$$

and a_B as:

$$a_B = \frac{\alpha}{4\pi R_\infty} = 5.29177210903 \times 10^{-11}\ \mathrm{m}. \tag{1.8}$$

α is a pure number equal to:

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{\mu_0 c e^2}{2h}, \tag{1.9}$$

where $\hbar = h/2\pi$, ϵ_0 the vacuum electric permittivity and μ_0 is the vacuum magnetic permeability. Hence the Bohr radius can be rewritten as:

$$a_B = \frac{\hbar}{\alpha m_e c} = \frac{\hbar^2 4\pi\epsilon_0}{m_e e^2}. \tag{1.10}$$

Eq. 1.9 allows the calculation of μ_0 as:

$$\mu_0 = \frac{2h\alpha}{e^2 c} = 1.25663706212 \times 10^{-6}\ \frac{\mathrm{N}}{\mathrm{A}^2}. \tag{1.11}$$

ϵ_0 is obtained from the relation:

$$\epsilon_0 = \frac{1}{\mu_0 c^2} = 8.8541878128 \times 10^{-12}\ \frac{\mathrm{C}^2}{\mathrm{N}\cdot\mathrm{m}^2}. \tag{1.12}$$

It is also useful to define the hartree energy:

$$E_h = \frac{e^2}{4\pi\epsilon_0 a_B} = 2hcR_\infty = 4.3597447222072 \times 10^{-18}\ \mathrm{J}, \tag{1.13}$$

and the Bohr magneton:

$$\mu_B = \frac{\hbar e}{2m_e} = 9.2740100783 \times 10^{-24}\ \mathrm{J/T}. \tag{1.14}$$

Chapter 2

Mechanical quantities

2.1 Time

In the SI, the unit of time is the second (symbol s), defined requiring that the frequency of a particular line of the ^{133}Cs atom is exactly $9192631770\ \mathrm{s}^{-1}$.

In a.u. the unit of time (symbol $\bar{\mathrm{t}}$) is defined requiring that the numerical value of $\hbar$ is 1. The conversion factor with the SI unit is obtained recalling that in the SI the Planck constant is $\hbar = \tilde{\hbar}\ \mathrm{J}\cdot\mathrm{s} = \tilde{\hbar}\ \mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}$. Therefore in a.u. we have:

$$\hbar = \frac{\bar{\mathrm{m}}\cdot\bar{\mathrm{l}}^2}{\bar{\mathrm{t}}}, \tag{2.1}$$

where $\bar{\mathrm{l}}$ is the unit of length and $\bar{\mathrm{m}}$ the unit of mass. As we discuss below $\bar{\mathrm{l}} = a_B$ and $\bar{\mathrm{m}} = m_e$, therefore

$$\bar{\mathrm{t}} = \frac{m_e a_B^2}{\hbar} = \frac{\hbar 4\pi\epsilon_0 a_B}{e^2} = \frac{\hbar}{E_h} = \frac{1.0545718176462\times10^{-34}\ \mathrm{J}\cdot\mathrm{s}}{4.3597447222072\times10^{-18}\ \mathrm{J}} = 2.41888843265857\times10^{-17}\ \mathrm{s} \tag{2.2}$$

In the c.g.s. system the unit of time is the second (symbol s), defined as in the SI. We have $\bar{\mathrm{t}}_{\mathrm{cgs}} = \mathrm{s}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{t}} = 2.41888843265857\times 10^{-17}\ \mathrm{s}$.

2.2 Length

In the SI, the unit of length is the metre (symbol m) defined as the length of the path traveled by light during the time interval of $1/299792458\ \mathrm{s}$.

In a.u. the unit of the length (symbol $\bar{\mathrm{l}}$) is defined requiring that the Bohr radius $a_B = \bar{\mathrm{l}}$. The conversion factor with the SI unit is $\bar{\mathrm{l}} = 5.29177210903 \times 10^{-11}\ \mathrm{m}$.

In the c.g.s. system the unit of length is the centimetre (symbol cm) defined as $\mathrm{cm} = 1.0 \times 10^{-2}\ \mathrm{m}$. We have $\bar{\mathrm{l}}_{\mathrm{cgs}} = 10^{-2}\ \mathrm{m}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{l}} = 5.29177210903 \times 10^{-9}\ \mathrm{cm}$.

A common unit of length is the angstrom (symbol Å). We have Å$= 10^{-10}\ \mathrm{m}$.

2.3 Mass

In the SI the unit of mass is the kilogram (symbol kg) defined requiring that the Planck constant h has the value $6.62607015 \times 10^{-34}\ \mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}$.

In a.u. the unit of mass (symbol $\bar{\mathrm{m}}$) is defined requiring that the mass of the electron $m_e = \bar{\mathrm{m}}$. The conversion factor with the SI unit is $\bar{\mathrm{m}} = 9.1093837015 \times 10^{-31}\ \mathrm{kg}$.

In the c.g.s. system the unit of mass is the gram (symbol g) defined as $\mathrm{g} = 1.0 \times 10^{-3}\ \mathrm{kg}$.

The conversion factor between the a.u. and the c.g.s. unit is $\bar{\mathrm{m}} = 9.1093837015 \times 10^{-28}\ \mathrm{g}$.

Atomic weights are usually expressed in atomic mass units ($\mathrm{a.m.u.} = 1.66053906660 \times 10^{-27}\ \mathrm{kg}$). This quantity can be converted in a.u. as:

$$\mathrm{a.m.u.} = \frac{1.66053906660 \times 10^{-27}\ \mathrm{kg}}{9.1093837015 \times 10^{-31}\ \mathrm{kg}}\ \bar{\mathrm{m}} = 1.8228884862 \times 10^{3}\ \bar{\mathrm{m}} \tag{2.3}$$

2.4 Mass density

In the SI the unit of mass density is derived from its definition:

$$\rho_m = \frac{dm}{dV}, \tag{2.4}$$

and it is $\mathrm{kg/m^3}$.

In a.u. the unit of mass density (symbol $\bar{\rho}_\mathrm{m}$) is derived from its definition: $\bar{\rho}_\mathrm{m} = \frac{\bar{\mathrm{m}}}{\bar{\mathrm{l}}^3}$. The conversion factor with the SI unit is:

$$\bar{\rho}_\mathrm{m} = \frac{m_e}{a_B^3} = \frac{9.1093837015 \times 10^{-31}\ \mathrm{kg}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^3} = 6.1473168257\ \mathrm{kg/m^3}. \tag{2.5}$$

In the c.g.s. system the unit of mass density is derived from its definition: $\mathrm{g/cm^3}$. The conversion factor with the SI unit is $\mathrm{g/cm^3} = 10^3\ \mathrm{kg/m^3}$.

The conversion factor between the a.u. and the c.g.s. unit is $\bar{\rho}_\mathrm{m} = 6.1473168257 \times 10^{-3}\ \mathrm{g/cm^3}$.

2.5 Frequency

In the SI the unit of frequency (symbol Hz) is the inverse of the unit of time: $\mathrm{Hz} = 1/\mathrm{s}$. This unit is called hertz. The angular frequency is defined as $\omega = 2\pi\nu$ where ν is the frequency. Its units are $\mathrm{radiant/s}$.

In a.u. the unit of frequency (symbol $\bar{\nu}$) is defined in a similar way $\bar{\nu} = 1/\bar{t}$. The conversion factor with the SI unit is:

$$\bar{\nu} = \frac{1}{2.4188843265857 \times 10^{-17}\ \mathrm{s}} = 4.1341373335182 \times 10^{16}\ \mathrm{Hz}. \tag{2.6}$$

In the c.g.s. system the unit of frequency is the hertz defined as in the SI.

The conversion factor between the a.u. and the c.g.s. unit is $\bar{\nu} = 4.1341373335182 \times 10^{16}\ \mathrm{Hz}$.

A commonly used unit of frequency is the wavenumber, that is the number of light waves with frequency ν per cm. If the wavelength λ is given in cm, the wavenumber is $\bar{\nu} = \frac{1}{\lambda}$ and its units are cm^{-1}. Since $\lambda = \frac{c}{\nu}$ the conversion factor from Hz to cm^{-1} is:

$$\frac{1}{10^2 c} = 3.33564095198152 \times 10^{-11}\ \mathrm{cm}^{-1}/\mathrm{Hz}, \tag{2.7}$$

while the conversion factor from cm^{-1} to Hz is:

$$10^2 c = 2.99792458 \times 10^{10}\ \mathrm{Hz/cm}^{-1} \tag{2.8}$$

2.6 Speed

In the SI the unit of speed is derived from its definition. For instance, the speed ($\mathbf{v}$) of a particle whose position as a function of time is $\mathbf{r}(t)$, is:

$$\mathbf{v} = \frac{d\mathbf{r}}{dt}, \tag{2.9}$$

so the unit of speed is $\mathrm{m/s}$.

In a.u. the unit of speed ($\bar{\mathrm{v}}$) is derived from its definition $\bar{\mathrm{v}} = \bar{\mathrm{l}}/\bar{\mathrm{t}}$. The conversion factor with the SI unit is:

$$\begin{aligned}\bar{\mathrm{v}} = \frac{a_B \hbar}{m_e a_B^2} = \frac{\hbar}{m_e a_B} = \alpha c &= 7.2973525693 \times 10^{-3}\ 2.99792458 \times 10^{8}\ \mathrm{m/s} \\ &= 2.18769126364 \times 10^{6}\ \mathrm{m/s}.\end{aligned} \tag{2.10}$$

Using the definitions of $\bar{\mathrm{l}}$ and $\bar{\mathrm{t}}$ we can also write:

$$\bar{\mathrm{v}} = \frac{a_B E_h}{\hbar}. \tag{2.11}$$

Note that since $\bar{\mathrm{v}} = \alpha c$ we can also write $c = \frac{1}{\alpha}\bar{\mathrm{v}}$ meaning that the speed of light in a.u. $c_{a.u.} = \frac{1}{\alpha} = 1.37035999084 \times 10^{2}$.

In the c.g.s. system the unit of speed is the $\bar{\mathrm{v}}_{\mathrm{cgs}} = \mathrm{cm/s} = 1.0 \times 10^{-2}\ \mathrm{m/s}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{v}} = 2.18769126364 \times 10^{8}\ \mathrm{cm/s}$.

2.7 Acceleration

In the SI the unit of acceleration is derived from its definition. For instance, the acceleration (a) of a particle whose position as a function of time is $\mathbf{r}(t)$, is:

$$\mathbf{a} = \frac{d^2\mathbf{r}}{dt^2}, \tag{2.12}$$

so the unit of acceleration is $\mathrm{m/s^2}$.

In a.u. the unit of acceleration ($\bar{\mathrm{a}}$) is derived from its definition $\bar{\mathrm{a}} = \bar{\mathrm{l}}/\bar{\mathrm{t}}^2$. The conversion factor with the SI unit is:

$$\begin{aligned}\bar{\mathrm{a}} = \frac{\bar{v}}{\bar{t}} = \frac{E_h \alpha c}{\hbar} &= \frac{4.3597447222072 \times 10^{-18}\ \mathrm{J}\ 7.2973525693 \times 10^{-3}\ 2.99792458 \times 10^{8}\ \mathrm{m/s}}{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}} \\ &= 9.0442161272 \times 10^{22}\ \mathrm{m/s^2}. \end{aligned} \tag{2.13}$$

In the c.g.s. system the unit of acceleration is the $\bar{\mathrm{a}}_{\mathrm{cgs}} = \mathrm{cm/s^2} = 1.0 \times 10^{-2}\ \mathrm{m/s^2}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{a}} = 9.0442161272 \times 10^{24}\ \mathrm{cm/s^2}$.

2.8 Momentum

In the SI the unit of momentum is derived from its definition. For instance, the momentum (**p**) of a particle of mass m whose position as a function of time is $\mathbf{r}(t)$, is:

$$\mathbf{p} = m\frac{d\mathbf{r}}{dt}, \tag{2.14}$$

so the unit of momentum is $\mathrm{kg} \cdot \mathrm{m/s}$.

In a.u. the unit of momentum ($\bar{\mathrm{p}}$) is derived from its definition $\bar{\mathrm{p}} = \bar{\mathrm{m}} \cdot \bar{\mathrm{v}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{p}} = \frac{m_e a_B}{\bar{\mathrm{t}}} = \frac{\hbar}{a_B} = \frac{1.0545718176462 \times 10^{-34}\ \mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}}{5.29177210903 \times 10^{-11}\ \mathrm{m}} = 1.99285191410 \times 10^{-24}\ \mathrm{kg} \cdot \mathrm{m/s}. \tag{2.15}$$

In the c.g.s. system the unit of momentum is $\bar{\mathrm{p}}_{\mathrm{cgs}} = \mathrm{g} \cdot \mathrm{cm/s} = 1.0 \times 10^{-5}\ \mathrm{kg} \cdot \mathrm{m/s}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{p}} = 1.99285191410 \times 10^{-19}\ \mathrm{g} \cdot \mathrm{cm/s}$.

2.9 Angular momentum

In the SI the unit of angular momentum is derived from its definition. For instance, the angular momentum ($\mathbf{L}$) of a particle at position $\mathbf{r}$ and with momentum $\mathbf{p}$ is:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{2.16}$$

so the unit of angular momentum is $\mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}$.

In a.u. the unit of angular momentum ($\bar{\mathrm{L}}$) is derived from its definition $\bar{\mathrm{L}} = \frac{\bar{\mathrm{m}} \cdot \bar{\mathrm{l}}^2}{\bar{\mathrm{t}}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{L}} = \frac{m_e a_B^2 \hbar}{m_e a_B^2} = \hbar = 1.0545718176462 \times 10^{-34}\ \mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}. \tag{2.17}$$

In the c.g.s. system the unit of angular momentum is $\bar{\mathrm{L}}_{\mathrm{cgs}} = \mathrm{g} \cdot \mathrm{cm}^2/\mathrm{s} = 1.0 \times 10^{-7}\ \mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{L}} = 1.0545718176462 \times 10^{-27}\ \mathrm{g} \cdot \mathrm{cm}^2/\mathrm{s}$.

2.10 Force

In the SI the unit of force (symbol N) is derived from the Newton equation:

$$\mathbf{F} = m\mathbf{a}, \tag{2.18}$$

so the unit of force is $\mathrm{N} = \mathrm{kg} \cdot \mathrm{m/s}^2$. This unit is called newton.

In a.u. the unit of force ($\bar{\mathrm{f}}$) is derived from the same equation so we have $\bar{\mathrm{f}} = \bar{\mathrm{m}} \cdot \bar{\mathrm{a}}$. The conversion factor with the SI unit is:

$$\begin{aligned}\bar{\mathrm{f}} &= \frac{m_e a_B \hbar E_h}{m_e a_B^2 \hbar} = \frac{E_h}{a_B} = \frac{4.3597447222072 \times 10^{-18}\mathrm{J}}{5.29177210903 \times 10^{-11}\mathrm{m}} \\ &= 8.2387234982 \times 10^{-8}\ \mathrm{N}.\end{aligned} \tag{2.19}$$

So in a.u. the unit of force is hartree/bohr.

In the c.g.s. system the unit of force is the $\bar{\mathrm{f}}_{\mathrm{cgs}} = \mathrm{g} \cdot \mathrm{cm/s}^2 = 1.0 \times 10^{-5}\ \mathrm{kg} \cdot \mathrm{m/s}^2$. This unit is called dyne.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{f}} = 8.2387234982 \times 10^{-3}\ \mathrm{dyne}$.

2.11 Energy

In the SI the unit of energy (symbol J) is derived from the definition of work:

$$U = \int \mathbf{F} \cdot d\mathbf{r} \tag{2.20}$$

so the unit of energy is $\mathrm{J} = \mathrm{kg} \cdot \mathrm{m}^2/\mathrm{s}^2 = \mathrm{N} \cdot \mathrm{m}$. This unit is called joule.

In a.u. the unit of energy ($\bar{\mathrm{U}}$) is derived from the definition of work so $\bar{\mathrm{U}} = \bar{\mathrm{f}} \cdot \bar{\mathrm{l}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{U}} = \frac{E_h}{a_B} a_B = E_h = 4.3597447222072 \times 10^{-18}\ \mathrm{J}, \tag{2.21}$$

so in a.u. the unit of the energy is the hartree.

In the c.g.s. system the unit of energy (symbol erg) is $\bar{\mathrm{U}}_{\mathrm{cgs}} = \mathrm{erg} = \mathrm{dyne} \cdot \mathrm{cm} = 1.0 \times 10^{-7}\ \mathrm{N} \cdot \mathrm{m}$. This unit is called erg.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{U}} = 4.3597447222072 \times 10^{-11}\ \mathrm{erg}$.

2.12 Power

In the SI the unit of power (symbol W) is derived from its definition as the work per unit time:

$$P = \frac{dU}{dt}, \tag{2.22}$$

so the unit of power is $\mathrm{W} = \mathrm{J/s}$. This unit is called watt.

In a.u. the unit of power ($\bar{\mathrm{W}}$) is derived from its definition $\bar{\mathrm{W}} = \frac{\bar{\mathrm{U}}}{\bar{\mathrm{t}}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{W}} = \frac{4.3597447222072 \times 10^{-18}\ \mathrm{J}}{2.4188843265857 \times 10^{-17}\ \mathrm{s}} = 1.8023783420686 \times 10^{-1}\ \mathrm{W}. \tag{2.23}$$

Using the definition of $\bar{\mathrm{t}}$ and $\bar{\mathrm{U}}$ we can also write:

$$\bar{\mathrm{W}} = \frac{E_{\hbar}^2}{\hbar}. \tag{2.24}$$

In the c.g.s. system the unit of power is $\bar{\mathrm{W}}_{\mathrm{cgs}} = \mathrm{erg/s} = 1.0 \times 10^{-7}\ \mathrm{W}$.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\mathrm{W}} = 1.8023783420686 \times 10^{6}\ \mathrm{erg/s}$.

2.13 Pressure

In the SI the unit of pressure (or stress) (symbol Pa) is derived from its definition as a force per unit area, so the unit of pressure is $\mathrm{N/m^2} = \mathrm{Pa}$. This unit is called pascal.

In a.u. the unit of pressure ($\bar{\sigma}$) is derived from its definition so $\bar{\sigma} = \frac{\bar{\mathrm{f}}}{\bar{\mathrm{l}}^2}$. The conversion factor with the SI unit is:

$$\bar{\sigma} = \frac{8.2387234982 \times 10^{-8}\ \mathrm{N}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^2} = 2.9421015696 \times 10^{13}\ \mathrm{Pa} \tag{2.25}$$

Note also that $\bar{\mathrm{f}} = \frac{E_h}{a_B}$ so $\bar{\sigma} = \frac{E_h}{a_B^3}$.

In the c.g.s. system the unit of pressure (symbol Ba) is the $\bar{\sigma}_{\mathrm{cgs}} = \mathrm{Ba} = \mathrm{dyne/cm^2} = 1.0 \times 10^{-1}\ \mathrm{Pa}$. This unit is called barye.

The conversion factor between the a.u. and the c.g.s. unit is: $\bar{\sigma} = 2.9421015696 \times 10^{14}\ \mathrm{Ba}$.

Other common units of pressure are: $\mathrm{bar} = 10^5\ \mathrm{Pa}$, atmosphere ($\mathrm{atm} = 1.01325\ \mathrm{bar}$), $\mathrm{torr} = \frac{1}{760}\ \mathrm{bar}$, millimeters of mercury ($\mathrm{mmHg} = 1\ \mathrm{torr}$).

2.14 Temperature

In the SI the unit of temperature is the kelvin (symbol K) defined so that the Boltzmann constant is $1.380649 \times 10^{-23}\mathrm{J/K}$.

In a.u. the unit of temperature (symbol K) is the kelvin as in the SI.

In the c.g.s. system the unit of temperature (symbol K) is the kelvin as in the SI.

In the SI the Avogadro number is exact and given by:

$$N_A = 6.02214076 \times 10^{23}, \tag{2.26}$$

and the universal gas constant is

$$R = k_B N_A = 1.380649 \times 10^{-23}\,\frac{\mathrm{J}}{\mathrm{K}} \times 6.02214076 \times 10^{23} = 8.31446261815324\,\frac{\mathrm{J}}{\mathrm{K}}. \tag{2.27}$$

The heat necessary to increase the temperature of water from 16.5 °C to 17.5 °C is known as (thermochemical) calorie (symbol cal) and is equal to 4.184 J. This is the definition that we use in `thermo_pw`. There is also another definition of calorie called international calorie and equal to 4.1868 J, but we do not use it.

Chapter 3

Electromagnetic quantities

3.1 Current

In the SI the unit of current is the ampere (symbol A) defined requiring that the charge of the electron is $e = 1.602176634 \times 10^{-19}\ \mathrm{A \cdot s}$. The quantity $\mathrm{A \cdot s}$ is called coulomb (symbol C).

In a.u. the unit of the current (symbol $\bar{\mathrm{I}}$) is derived from its definition:

$$I = \frac{dq}{dt}, \tag{3.1}$$

where dq is the charge that passes through a cross section of the conductor in the time dt, so $\bar{\mathrm{I}} = \bar{\mathrm{C}}/\bar{\mathrm{t}}$ where $\bar{\mathrm{C}}$ is the unit of charge (equal to e, see below). The conversion factor with the SI unit is:

$$\bar{\mathrm{I}} = \frac{eE_h}{\hbar} = \frac{1.602176634 \times 10^{-19}\ \mathrm{C}\ 4.3597447222072 \times 10^{-18}\mathrm{J}}{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}} = 6.623618237510 \times 10^{-3}\mathrm{A}. \tag{3.2}$$

In the c.g.s.-Gaussian system the unit of current (symbol statA) is defined from Ampère law. The force per unit length between two parallel wires that carry a current I and I' is:

$$\frac{F}{l} = \frac{2}{c^2}\frac{II'}{r}, \tag{3.3}$$

therefore $\bar{\mathrm{I}}_{\mathrm{cgs}} = \mathrm{statA} = \sqrt{\mathrm{dyne}}\ \mathrm{cm/s}$. This unit is called statampere or electrostatic unit (esu) of current.

In order to convert between statA and A, we can write $\mathrm{A} = \mathcal{K}\ \mathrm{statA}$. When the currents in the two wires are $I\ \mathrm{statA} = \frac{I}{\mathcal{K}}\mathrm{A}$ and $I'\ \mathrm{statA} = \frac{I'}{\mathcal{K}}\mathrm{A}$ and their distance is $r\ \mathrm{cm} = r\ 10^{-2}\ \mathrm{m}$ the force per metre is in $\mathrm{N/m} = \frac{10^5}{10^2}\mathrm{dyne/cm}$

$$F = 2\frac{\tilde{\mu}_0}{4\pi}\frac{10^3}{10^{-2}\mathcal{K}^2}\ \frac{I\ I'}{r}\mathrm{dyne/cm}, \tag{3.4}$$

where $\tilde{\mu}_0$ is the numerical value of μ_0 in SI units (see Eq. 1.11). Comparing this equation with Eq. 3.3 we obtain:

$$\frac{\tilde{\mu}_0}{4\pi}\frac{10^5}{\mathcal{K}^2} = \frac{1}{\tilde{c}_{cgs}^2}, \tag{3.5}$$

where $\tilde{c}_{cgs}$ is the numerical value of the speed of light in c.g.s. units. We have $\tilde{c}_{cgs} = 10^2\tilde{c}$ where $\tilde{c}$ is the numerical value of the speed of light in SI units. From this equation we obtain:

$$\mathcal{K} = \tilde{c}_{cgs}\sqrt{\frac{10^5\tilde{\mu}_0}{4\pi}} = \frac{\tilde{c}_{cgs}}{\tilde{c}}\sqrt{\frac{10^5}{4\pi\tilde{\epsilon}_0}} = \sqrt{\frac{10^9}{4\pi\tilde{\epsilon}_0}} = 2.99792458082 \times 10^9, \tag{3.6}$$

where $\tilde{\epsilon}_0$ is the numerical value of the vacuum permittivity in SI units (Eq. 1.12).
In the old SI units $\frac{\tilde{\mu}_0}{4\pi} = 10^{-7}$, so $\mathcal{K} = 10^{-1}\tilde{c}_{cgs} = 10\ \tilde{c}$. In the new SI we have:

$$\frac{\mathcal{K}}{10\tilde{c}} = 1.00000000027... \tag{3.7}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{I}} = 6.623618237510 \times 10^{-3}\ \mathcal{K}\ \mathrm{statA} = 1.98571079282 \times 10^7\ \mathrm{statA}$.

3.2 Charge

In the SI the unit of the charge (symbol C), derived from the definition of the current:

$$I = \frac{dq}{dt}, \tag{3.8}$$

is the charge that passes in one second through the section of a conductor in which the current is $1\mathrm{A}$. This unit is called coulomb.

In the SI the Coulomb force between two charges q and q' at distance $\mathbf{r}$ is:

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0}\frac{q\,q'}{r^3}\,\mathbf{r}, \tag{3.9}$$

where $r = |\mathbf{r}|$.

In a.u. the unit of the charge (symbol $\bar{\mathrm{C}}$) is defined requiring that the electron has charge $e = \bar{\mathrm{C}}$. The conversion factor between a.u. and the SI unit is:

$$\bar{\mathrm{C}} = 1.602176634 \times 10^{-19}\ \mathrm{C}. \tag{3.10}$$

With this information we can derive the form of the Coulomb law in a.u.. A charge $q\ \bar{\mathrm{C}}$ at a distance $r\ \bar{\mathrm{l}}$ from a charge $q'\ \bar{\mathrm{C}}$ will fill a force $F\bar{\mathrm{f}}$ that can be calculated using Eq. 3.9:

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0}\frac{\bar{\mathrm{C}}^2}{\bar{\mathrm{l}}^2\bar{\mathrm{f}}}\frac{q\,q'}{r^3}\,\mathbf{r}, \tag{3.11}$$

but since

$$\frac{1}{4\pi\epsilon_0}\frac{\bar{\mathrm{C}}^2}{\bar{\mathrm{l}}^2\bar{\mathrm{f}}} = \frac{E_h}{a_B\bar{\mathrm{f}}} = 1 \tag{3.12}$$

the Coulomb law in a.u. is:

$$\mathbf{F} = \frac{q\,q'}{r^3}\,\mathbf{r}. \tag{3.13}$$

In the c.g.s. system the unit of charge (symbol statC) is defined from the Coulomb law:

$$\mathbf{F} = \frac{q\,q'}{r^3}\,\mathbf{r}, \tag{3.14}$$

Therefore the charge unit is $\bar{\mathrm{C}}_{\mathrm{cgs}} = \mathrm{statC} = \sqrt{\mathrm{dyne}}\cdot\mathrm{cm} = \mathrm{statA}\cdot\mathrm{s}$. This unit is called statcoulomb or electrostatic unit (esu) of charge or franklin.

The conversion factor between statC and C can be found by writing $\mathrm{statC} = \frac{1}{\mathcal{K}}\mathrm{C}$ and considering two charges of $q\ \mathrm{statC}$ and $q'\ \mathrm{statC}$ respectively, at a distance of $r\ \mathrm{cm}$. Since the two charges are of $\frac{q}{\mathcal{K}}\ \mathrm{C}$ and $\frac{q'}{\mathcal{K}}\ \mathrm{C}$ at the distance of r 10^{-2} m, we can use the Coulomb law in SI units to find the force (in $\mathrm{N} = 10^5\mathrm{dyne}$) acting between them:

$$\mathbf{F} = \frac{1}{4\pi\tilde{\epsilon}_0}\frac{10^5}{10^{-4}\mathcal{K}^2}\frac{q\,q'}{r^3}\,\mathbf{r}\ \mathrm{dyne} \tag{3.15}$$

and comparing this equation with Eq. 3.14 we find:

$$\mathcal{K} = \sqrt{\frac{10^9}{4\pi\tilde{\epsilon}_0}} = 2.99792458082 \times 10^9. \tag{3.16}$$

Using this conversion factor we can write the equation that defines the current. When a charge dq statC, or $\frac{dq}{\mathcal{K}}$ C passes in dt s through a section of a conductor, the current (due to Eq. 3.8) is $I = \frac{1}{\mathcal{K}}\frac{dq}{dt}$ A $= \frac{dq}{dt}$ statA, so in the c.g.s.-Gaussian system Eq. 3.8 still holds.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{C}} = 1.602176634 \times 10^{-19}\ \mathcal{K}\ \mathrm{statC} = 4.80320471388 \times 10^{-10}\ \mathrm{statC}$.

3.3 Charge density

In the SI the unit of the charge density is derived from its definition:

$$\rho = \frac{dq}{dV}, \tag{3.17}$$

so the unit of the charge density is $\mathrm{C/m^3}$.

In a.u. the unit of charge density (symbol $\bar{\rho}$) is derived its definition $\bar{\rho} = \frac{\bar{\mathrm{C}}}{\bar{\mathrm{l}}^3}$. The conversion factor with the SI unit is:

$$\bar{\rho} = \frac{e}{a_B^3} = \frac{1.602176634 \times 10^{-19}\ \mathrm{C}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^3} = 1.08120238456 \times 10^{12}\ \mathrm{C/m^3}. \tag{3.18}$$

In the c.g.s. system the unit of charge density is derived from its definition and it is $\bar{\rho}_{\mathrm{cgs}} = \mathrm{statC/cm^3} = \frac{1}{\mathcal{K}\ 10^{-6}}\ \mathrm{C/m^3} = 3.33564095107 \times 10^{-4}\ \mathrm{C/m^3}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\rho} = 3.2413632055 \times 10^{15}\ \mathrm{statC/cm^3}$.

3.4 Current density

In the SI the unit of the current density is derived from its definition:

$$I = \int \mathbf{J} \cdot \hat{\mathbf{n}} \, dS, \tag{3.19}$$

so the unit of the current density is $\mathrm{A/m^2}$.
In SI units the continuity equation is:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}. \tag{3.20}$$

In a.u. the unit of the current density (symbol $\bar{\mathrm{J}}$) is derived from the same equation so we have $\bar{\mathrm{J}} = \frac{\bar{\mathrm{I}}}{\bar{\mathrm{l}}^2}$. The conversion factor to SI units is:

$$\bar{\mathrm{J}} = \frac{6.623618237510 \times 10^{-3}\ \mathrm{A}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^2} = 2.36533701094 \times 10^{18}\ \mathrm{A/m^2}. \tag{3.21}$$

Inserting the expressions of $\bar{\mathrm{I}}$ and $\bar{\mathrm{l}}$ we can also write:

$$\bar{\mathrm{J}} = \frac{eE_h}{\hbar a_B^2}. \tag{3.22}$$

The continuity equation can be written as:

$$\frac{\partial \rho}{\partial t} = -\frac{\bar{\mathrm{t}}\bar{\mathrm{J}}}{\bar{\rho}\bar{\mathrm{l}}} \nabla \cdot \mathbf{J}. \tag{3.23}$$

Since $\frac{\bar{\mathrm{t}}\bar{\mathrm{J}}}{\bar{\rho}\bar{\mathrm{l}}} = 1$ the continuity equation is Eq. 3.20.

In the c.g.s.-Gaussian system the unit of current density (symbol $\bar{\mathrm{J}}_{\mathrm{cgs}}$) is derived from its definition $\bar{\mathrm{J}}_{\mathrm{cgs}} = \mathrm{statA/cm^2} = \frac{1}{\mathcal{K}10^{-4}}\mathrm{A/m^2} = 3.33564095107 \times 10^{-6}\ \mathrm{A/m^2}$. Since in Eq. 3.23 $\frac{\bar{\mathrm{t}}_{\mathrm{cgs}}\bar{\mathrm{J}}_{\mathrm{cgs}}}{\bar{\rho}_{\mathrm{cgs}}\bar{\mathrm{l}}_{\mathrm{cgs}}} = 1$ the continuity equation is Eq. 3.20.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{J}} = 7.0911019670 \times 10^{23}\ \mathrm{statA/cm^2}$

3.5 Electric field

In the SI the unit of the electric field is derived from its definition:

$$\mathbf{E} = \frac{\mathbf{F}}{q}, \tag{3.24}$$

so the unit of the electric field is $\mathrm{N/C} = \frac{\mathrm{kg \cdot m}}{\mathrm{s^2 \cdot C}} = \mathrm{V/m}$.

In a.u. the unit of the electric field (symbol $\bar{\mathrm{E}}$) is derived from its definition $\bar{\mathrm{E}} = \frac{\bar{\mathrm{f}}}{\bar{\mathrm{C}}}$. The conversion factor to the SI unit is:

$$\bar{\mathrm{E}} = \frac{E_h}{a_B e} = \frac{8.2387234982 \times 10^{-8}\ \mathrm{N}}{1.602176634 \times 10^{-19}\ \mathrm{C}} = 5.14220674763 \times 10^{11}\ \mathrm{N/C}. \tag{3.25}$$

In the c.g.s.-Gaussian system the unit of electric field (symbol $\mathrm{statV/cm}$) is derived from its definition: $\bar{\mathrm{E}}_{\mathrm{cgs}} = \mathrm{statV/cm} = \mathrm{dyne/statC} = 10^{-5}\ \mathcal{K}\ \mathrm{N/C} = 2.99792458082 \times 10^4\ \mathrm{N/C}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{E}} = 1.71525554062 \times 10^7\ \mathrm{statV/cm}$.

3.6 Electric potential

In the SI the unit of the electric potential (symbol V) is derived from its definition. The electric potential is a function $\phi(\mathbf{r})$ such that:

$$\mathbf{E} = -\nabla\phi(\mathbf{r}), \tag{3.26}$$

so the unit of the electric potential is $\mathrm{V} = \frac{\mathrm{N \cdot m}}{\mathrm{C}} = \frac{\mathrm{J}}{\mathrm{C}}$. This unit is called volt.

In a.u. the unit of the electric potential (symbol $\bar{\mathrm{V}}$) is derived from its definition so $\bar{\mathrm{V}} = \bar{\mathrm{E}} \cdot \bar{\mathrm{l}}$. The conversion factor to the SI unit is:

$$\bar{\mathrm{V}} = \frac{E_h}{e} = \frac{4.3597447222072 \times 10^{-18}\ \mathrm{N \cdot m}}{1.602176634 \times 10^{-19}\ \mathrm{C}} = 2.7211386245988 \times 10^{1}\ \mathrm{V}. \tag{3.27}$$

In the c.g.s.-Gaussian system the unit of electric potential (symbol statV) is derived from its definition: $\bar{\mathrm{V}}_{\mathrm{cgs}} = \mathrm{statV} = \mathrm{dyne \cdot cm/statC} = 10^{-7}\ \mathcal{K}\ \mathrm{N \cdot m/C} = 2.99792458082 \times 10^{2}\ \mathrm{V}$. This unit is called statvolt. Note that $\mathrm{statV} = \sqrt{\mathrm{dyne}}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{V}} = 9.07674142975 \times 10^{-2}\ \mathrm{statV}$.

A commonly used unit of energy is the electron volt (symbol eV) defined as the energy acquired by an electron accelerated through a potential difference of $1\mathrm{V}$. Therefore $\mathrm{eV} = 1.602176634 \times 10^{-19}\ \mathrm{C \cdot V}$ (or J). The Hartree energy espressed in eV is:

$$E_h = 2.7211386245988 \times 10^{1}\ \mathrm{eV}, \tag{3.28}$$

while the Rydberg energy expressed in eV is:

$$\frac{E_h}{2} = 1.3605693122994 \times 10^{1}\ \mathrm{eV}. \tag{3.29}$$

These units are used also to measure the frequency giving the energy of a photon of frequency ν, that is $h\nu$ instead of ν.

3.7 Capacitance

In the SI the unit of the capacitance (symbol F) is derived from its definition. The capacitance of a capacitor is the ratio between the charge on its surfaces and the voltage applied between them:

$$C = q/V, \tag{3.30}$$

so the unit of the capacitance is $\mathrm{F} = \frac{\mathrm{C}}{\mathrm{V}} = \frac{\mathrm{A{\cdot}s}}{\mathrm{V}} = \frac{\mathrm{C}^2}{\mathrm{N{\cdot}m}} = \frac{\mathrm{C}^2}{\mathrm{J}}$. This unit is called farad.

In a.u. the unit of the capacitance (symbol $\bar{\mathrm{F}}$) is derived from its definition: $\bar{\mathrm{F}} = \frac{\bar{\mathrm{C}}}{\bar{\mathrm{V}}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{F}} = \frac{e^2}{E_h} = \frac{(1.602176634 \times 10^{-19}\ \mathrm{C})^2}{4.3597447222072 \times 10^{-18}\ \mathrm{J}} = 5.887890530517 \times 10^{-21}\ \mathrm{F}. \tag{3.31}$$

In the c.g.s.-Gaussian system the unit of capacitance is derived from its definition: $\bar{\mathrm{C}}_{\mathrm{cgs}} = \mathrm{statC}/\mathrm{statV} = \mathrm{cm}$. The conversion factor with the SI unit is: $\mathrm{cm} = \frac{1}{10^{-7}\ \mathcal{K}^2}\ \mathrm{C}/\mathrm{V} = 1.11265005544 \times 10^{-12}\ \mathrm{F}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{F}} = 5.29177210903 \times 10^{-9}\ \mathrm{cm}$.

3.8 Vacuum electric permittivity

In the SI the unit of the vacuum electric permittivity ϵ_0 can be derived from the Coulomb law:

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0}\frac{qq'}{r^3}\mathbf{r}, \tag{3.32}$$

so the unit of ϵ_0 is $\frac{\mathrm{C}^2}{\mathrm{N\cdot m}^2} = \frac{\mathrm{F}}{\mathrm{m}}$. Its numerical value in these units is given in Eq. 1.12.

In a.u. ϵ_0 is not used.

In the c.g.s.-Gaussian system ϵ_0 is not used.

In a.u. ϵ_0 is not used.

3.9 Electric dipole moment

In the SI the unit of the electric dipole moment of a localized charge density is derived from its definition:

$$\wp = \int_V \mathbf{r}\rho(\mathbf{r})d^3r, \tag{3.33}$$

so the units of the electric dipole moment are $\mathrm{C} \cdot \mathrm{m}$.

In a.u. the unit of electric dipole moment is derived from its definition $\bar{\wp} = \bar{\mathrm{C}} \cdot \bar{\mathrm{l}}$. The conversion factor to the SI unit is:

$$\bar{\wp} = e\,a_B = 1.602176634 \times 10^{-19}\ \mathrm{C}\ 5.29177210903 \times 10^{-11}\mathrm{m} = 8.4783536255 \times 10^{-30}\ \mathrm{C} \cdot \mathrm{m}. \tag{3.34}$$

In the c.g.s.-Gaussian system the unit of electric dipole is derived from its definition $\bar{\wp}_{\mathrm{cgs}} = \mathrm{statC} \cdot \mathrm{cm}$. The conversion factor to the SI unit is $\bar{\wp}_{\mathrm{cgs}} = \frac{10^{-2}}{\mathcal{K}}\ \mathrm{C} \cdot \mathrm{m} = 3.33564095107 \times 10^{-12}\ \mathrm{C} \cdot \mathrm{m}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\wp} = 2.54174647389 \times 10^{-18}\ \mathrm{statC} \cdot \mathrm{cm}$.

3.10 Polarization

In the SI the unit of the polarization is derived from its definition as the electric dipole per unit volume $\frac{\mathrm{C}}{\mathrm{m}^2}$:

$$\mathbf{P} = \wp/V. \tag{3.35}$$

In a.u. the unit of the polarization (symbol $\bar{\mathrm{P}}$) is derived from its definition $\bar{\mathrm{P}} = \frac{\bar{\mathrm{C}}}{\bar{\mathrm{l}}^2}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{P}} = \frac{e}{a_B^2} = \frac{1.602176634 \times 10^{-19}\ \mathrm{C}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^2} = 5.7214766229 \times 10^{1}\ \mathrm{C/m^2}. \tag{3.36}$$

In the c.g.s.-Gaussian system the unit of polarization is derived from its definition: $\bar{\mathrm{P}}_{\mathrm{cgs}} = \mathrm{statC/cm^2} = \frac{1}{\mathcal{K}\ 10^{-4}}\ \mathrm{C/m^2} = 3.33564095107 \times 10^{-6}\ \mathrm{C/m^2}$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{P}} = 1.71525554062 \times 10^{7}\ \mathrm{statC/cm^2}$.

3.11 Electric displacement

In the SI the electric displacement is given in term of the electric field and of the polarization by:

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \tag{3.37}$$

so the polarization and the electric displacement have the same unit $\frac{\mathrm{C}}{\mathrm{m}^2}$. This equation is usually justified starting from the Maxwell's equation:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{3.38}$$

and separating ρ into $\rho = \rho_f + \rho_b$ where ρ_f are the free charges and ρ_b are the bound charges such that:

$$\rho_b = -\nabla \cdot \mathbf{P}. \tag{3.39}$$

Therefore one obtains:

$$\nabla \cdot (\epsilon_0 \mathbf{E} + \mathbf{P}) = \rho_f. \tag{3.40}$$

In a.u. the unit of the electric displacement (symbol $\bar{\mathrm{D}}$) is derived from the relationship between electric displacement, electric field, and polarization that can be found writing the above equations in a.u.. The Maxwell's equation becomes:

$$\frac{\bar{\mathrm{E}}}{\bar{\mathrm{l}}} \nabla \cdot \mathbf{E} = \frac{\bar{\rho}}{\epsilon_0} \rho \tag{3.41}$$

and since $\frac{\bar{\rho} \cdot \bar{\mathrm{l}}}{\epsilon_0 \bar{\mathrm{E}}} = 4\pi$, in a.u. we have:

$$\nabla \cdot \mathbf{E} = 4\pi\rho. \tag{3.42}$$

The link between bound charges and polarization does not change:

$$\rho_b = -\frac{\bar{\mathrm{P}}}{\bar{\mathrm{l}} \cdot \bar{\rho}} \nabla \cdot \mathbf{P} = -\nabla \cdot \mathbf{P}, \tag{3.43}$$

where we used the fact that $\frac{\bar{\mathrm{P}}}{\bar{\mathrm{l}} \cdot \bar{\rho}} = 1$. Inserting this expression in the Maxwell's equation we obtain:

$$\nabla \cdot (\mathbf{E} + 4\pi \mathbf{P}) = 4\pi \rho_f, \tag{3.44}$$

that suggests the following definition of the electric displacement:

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P}. \tag{3.45}$$

Finally we can find $\bar{\mathrm{D}}$ by using Eq. 3.37 for an electric field $\mathbf{E}\bar{\mathrm{E}}$, a polarization $\mathbf{P}\bar{\mathrm{P}}$ and a displacement $\mathbf{D}\bar{\mathrm{D}}$:

$$\mathbf{D} = \left[\mathbf{E}\,\frac{\epsilon_0\bar{\mathrm{E}}}{\bar{\mathrm{D}}} + \mathbf{P}\frac{\bar{\mathrm{P}}}{\bar{\mathrm{D}}}\right]. \tag{3.46}$$

Comparing this equation with Eq. 3.45 we obtain:

$$\bar{\mathrm{D}} = \epsilon_0\bar{\mathrm{E}} = \frac{\bar{\mathrm{P}}}{4\pi} \tag{3.47}$$

or $\bar{\mathrm{D}} = \frac{\bar{\mathrm{P}}}{4\pi} = 4.5530064316\ \mathrm{C/m^2}$.

In the c.g.s.-Gaussian system the relationship between electric displacement, electric field, and polarization can be found noticing that in Eq. 3.41 $\frac{\bar{\rho}_{\mathrm{cgs}}\cdot\bar{\mathrm{l}}_{\mathrm{cgs}}}{\epsilon_0\bar{\mathrm{E}}_{\mathrm{cgs}}} = 4\pi$ so that the Maxwell's equation becomes:

$$\nabla\cdot\mathbf{E} = 4\pi\rho. \tag{3.48}$$

Moreover since $\frac{\bar{\mathrm{P}}_{\mathrm{cgs}}}{\bar{\mathrm{l}}_{\mathrm{cgs}}\cdot\bar{\rho}_{\mathrm{cgs}}} = 1$, the link between bound charge and polarization is as in the SI units and we obtain:

$$\nabla\cdot(\mathbf{E} + 4\pi\mathbf{P}) = 4\pi\rho_f, \tag{3.49}$$

that suggests the following relationship between electric displacement, electric field and polarization:

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}. \tag{3.50}$$

The conversion factor with the SI unit $\bar{\mathrm{D}}_{\mathrm{cgs}}$ can be found from Eq. 3.46 that compared with Eq. 3.50 gives:

$$\bar{\mathrm{D}}_{\mathrm{cgs}} = \epsilon_0\bar{\mathrm{E}}_{\mathrm{cgs}} = \frac{\bar{\mathrm{P}}_{\mathrm{cgs}}}{4\pi}. \tag{3.51}$$

The electric displacement and the polarization have the same dimensions $\mathrm{statC/cm^2}$ but while the unit of polarization is $\bar{\mathrm{P}}_{\mathrm{cgs}} = 1\ \mathrm{statC/cm^2}$ the unit of electric displacement is $\bar{\mathrm{D}}_{\mathrm{cgs}} = \frac{1}{4\pi}\ \mathrm{statC/cm^2}$. The conversion factor to SI units is:

$$\bar{\mathrm{D}}_{\mathrm{cgs}} = \frac{1}{4\pi\ \mathcal{K}\ 10^{-4}}\ \mathrm{C/m^2} = 2.65441872871\times10^{-7}\ \mathrm{C/m^2}. \tag{3.52}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{D}} = 1.71525554062\times10^{7}\ \mathrm{statC/(cm^2\cdot 4\pi)}$.

3.12 Resistance

In the SI the unit of the resistance (symbol Ω) is derived from its definition. The resistance is the ratio between the applied voltage and the current that passes through a system:

$$R = V/I, \tag{3.53}$$

so the unit of the resistance is $\Omega = \frac{\mathrm{V}}{\mathrm{A}} = \frac{\mathrm{N \cdot m \cdot s}}{\mathrm{C}^2} = \frac{\mathrm{J \cdot s}}{\mathrm{C}^2}$. This unit is called ohm.

In a.u. the unit of the resistance (symbol $\bar{\Omega}$) is derived from its definition: $\bar{\Omega} = \frac{\bar{\mathrm{V}}}{\bar{\mathrm{I}}}$. The conversion factor with the SI unit is:

$$\bar{\Omega} = \frac{E_h \hbar}{e^2 E_h} = \frac{\hbar}{e^2} = \frac{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}}{(1.602176634 \times 10^{-19}\ \mathrm{C})^2} = 4.1082359022277 \times 10^{3}\ \Omega. \tag{3.54}$$

In the c.g.s.-Gaussian system the unit of resistance is derived from its definition: $\bar{\Omega}_{\mathrm{cgs}} = \mathrm{statV/statA} = \mathrm{s/cm}$. The conversion factor with the SI unit is: $\bar{\Omega}_{\mathrm{cgs}} = 10^{-7}\ \mathcal{K}^2\ \mathrm{V/A} = 8.9875517923 \times 10^{11}\ \Omega$.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\Omega} = 4.57102890439 \times 10^{-9}\ \mathrm{s/cm}$.

3.13 Magnetic flux density

In the SI the unit of the magnetic flux density (symbol T) can be derived from the Lorentz force equation:

$$\mathbf{F} = q(\mathbf{v} \times \mathbf{B}), \tag{3.55}$$

so the unit of the magnetic flux density is $\mathrm{T} = \frac{\mathrm{N \cdot s}}{\mathrm{C \cdot m}} = \frac{\mathrm{V \cdot s}}{\mathrm{m^2}} = \frac{\mathrm{N}}{\mathrm{A \cdot m}} = \frac{\mathrm{kg}}{\mathrm{s \cdot C}}$. This unit is called tesla.
In the SI the second Maxwell's equation reads:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \tag{3.56}$$

In a.u. the unit of the magnetic flux density (symbol $\bar{\mathrm{B}}$) is derived from the Lorentz force: $\bar{\mathrm{B}} = \frac{\bar{\mathrm{f}}}{\bar{\mathrm{v}} \cdot \bar{\mathrm{C}}}$. The conversion factor with the SI unit is:

$$\begin{aligned}\bar{\mathrm{B}} = \frac{E_h \hbar}{a_B^2 E_h e} = \frac{\hbar}{a_B^2 e} &= \frac{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}}{(5.29177210903 \times 10^{-11}\ \mathrm{m})^2\ 1.602176634 \times 10^{-19}\ \mathrm{C}} \\ &= 2.35051756758 \times 10^5\ \mathrm{T}.\end{aligned} \tag{3.57}$$

Using the expression of a_B we can also write:

$$\bar{\mathrm{B}} = \frac{m_e e}{a_B \hbar 4\pi\epsilon_0} = \frac{E_h}{2\mu_B}, \tag{3.58}$$

where E_h is the Hartree energy (Eq.1.13) and μ_B is the Bohr magneton (Eq. 1.14). In these units the second Maxwell's equation is:

$$\nabla \times \mathbf{E} = -\frac{\bar{\mathrm{l}} \cdot \bar{\mathrm{B}}}{\bar{\mathrm{t}} \cdot \bar{\mathrm{E}}} \frac{\partial \mathbf{B}}{\partial t}. \tag{3.59}$$

Since $\frac{\bar{\mathrm{l}} \cdot \bar{\mathrm{B}}}{\bar{\mathrm{t}} \cdot \bar{\mathrm{E}}} = 1$, the second Maxwell's equation has the same form as in the SI.

In the c.g.s.-Gaussian system the unit of magnetic flux density (symbol G) is derived from the Ampère law by writing the force per unit length between two parallel wires traversed by a current I as:

$$\frac{F}{l} = \frac{1}{c} B \cdot I, \tag{3.60}$$

where $B = \frac{2}{c}\frac{I}{r}$ is the magnetic flux density produced by one wire at the distance of the other. This relationship shows that B has the dimensions of a charge per unit area $\mathrm{statC/cm^2}$. This unit is called gauss.
The conversion factor with the SI unit can be found using the expression of the magnetic flux density B produced by a wire crossed by a currenit I in

SI units: $B = \frac{\mu_0}{2\pi}\frac{I}{r}$. Writing $\mathrm{G} = \frac{1}{\mathcal{K}_T}\mathrm{T}$, a current of I statA $= \frac{I}{\mathcal{K}}\mathrm{A}$ produces at a distance of r $10^{-2}\mathrm{m}$ a magnetic field (in $\mathrm{T} = \mathcal{K}_T\mathrm{G}$):

$$B = \frac{\tilde{\mu}_0}{2\pi}\frac{\mathcal{K}_T}{10^{-2}\mathcal{K}}\frac{I}{r}\ \mathrm{G}. \tag{3.61}$$

Comparing with the c.g.s.-Gaussian expression we obtain:

$$\mathcal{K}_T = \frac{4\pi}{\tilde{\mu}_0}\frac{10^{-2}\ \mathcal{K}}{\tilde{c}_{cgs}} = \frac{10^3}{\mathcal{K}_A} = 9.99999999726 \times 10^3, \tag{3.62}$$

where $\mathcal{K}_A = \mathcal{K}/\tilde{c}_{cgs} = 1.000000000274 \times 10^{-1}$. With the old SI units $\mathcal{K}_T$ was exactly 10^4.
Using the conversion factor between T and G we can write the Lorentz force in the c.g.s-Gaussian system. A particle with charge q statC $= \frac{q}{\mathcal{K}}$ C that moves with a speed of $\mathbf{v}$ cm/s $= \mathbf{v}\ 10^{-2}$ m/s in a field of $\mathbf{B}$ G $= \frac{\mathbf{B}}{\mathcal{K}_T}$ T will fill a force (in $\mathrm{N} = 10^5$ dyne) (using Eq. 3.55):

$$\mathbf{F} = \frac{10^{-2}}{\mathcal{K}\ \mathcal{K}_T} q\ (\mathbf{v} \times \mathbf{B})\ 10^5\ \mathrm{dyne}. \tag{3.63}$$

Since $\frac{10^3}{\mathcal{K}\mathcal{K}_T} = \frac{1}{\tilde{c}_{cgs}}$ we obtain the Lorentz force in the c.g.s.-Gaussian system:

$$\mathbf{F} = \frac{q}{c}\ (\mathbf{v} \times \mathbf{B}). \tag{3.64}$$

The second Maxwell's equation can be found noticing that in Eq. 3.59 $\frac{\bar{\mathrm{l}}_{\mathrm{cgs}} \cdot \bar{\mathrm{B}}_{\mathrm{cgs}}}{\bar{\mathrm{t}}_{\mathrm{cgs}} \cdot \bar{\mathrm{E}}_{\mathrm{cgs}}} = \frac{10^{-2}}{\mathcal{K}_T 10^{-5}\mathcal{K}} = \frac{10^3\mathcal{K}_A}{10^3\mathcal{K}} = \frac{1}{\tilde{c}_{cgs}}$ so we have:

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}. \tag{3.65}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{B}} = 2.35051756693 \times 10^9$ G.

3.14 Vector potential

In the SI the unit of the vector potential (symbol $\mathrm{T} \cdot \mathrm{m}$) is derived from its definition. The vector potential (**A**) is a vector field such that:

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{3.66}$$

so the unit of the vector potential is $\mathrm{T} \cdot \mathrm{m} = \frac{\mathrm{N}}{\mathrm{A}} = \frac{\mathrm{V \cdot s}}{\mathrm{m}} = \frac{\mathrm{N \cdot s}}{\mathrm{C}}$.
When the vector potential depends on time the electric field is:

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}. \tag{3.67}$$

In a.u. the unit of the vector potential (symbol $\bar{\mathrm{A}}$) is derived from its definition $\bar{\mathrm{A}} = \bar{\mathrm{B}} \cdot \bar{\mathrm{l}}$. We have:

$$\begin{aligned}\bar{\mathrm{A}} = \frac{\hbar}{a_B e} &= \frac{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}}{5.29177210903 \times 10^{-11}\ \mathrm{m}\ 1.602176634 \times 10^{-19}\ \mathrm{C}} \\ &= 1.24384033059 \times 10^{-5}\ \mathrm{T \cdot m}.\end{aligned} \tag{3.68}$$

When the vector potential depends on time the electric field is:

$$\mathbf{E} = -\frac{\bar{\mathrm{V}}}{\bar{\mathrm{E}} \cdot \bar{\mathrm{l}}}\nabla\phi - \frac{\bar{\mathrm{A}}}{\bar{\mathrm{E}} \cdot \bar{\mathrm{t}}}\frac{\partial \mathbf{A}}{\partial t}. \tag{3.69}$$

Since $\frac{\bar{\mathrm{V}}}{\bar{\mathrm{E}} \cdot \bar{\mathrm{l}}} = 1$ and $\frac{\bar{\mathrm{A}}}{\bar{\mathrm{E}} \cdot \bar{\mathrm{t}}} = 1$ Eq. 3.67 holds also in a.u..

In the c.g.s.-Gaussian system the unit of the vector potential (symbol $\bar{\mathrm{A}}_{\mathrm{cgs}}$) is derived from its definition Eq. 3.66. The conversion factor with the SI unit is $\bar{\mathrm{A}}_{\mathrm{cgs}} = \mathrm{G} \cdot \mathrm{cm} = \frac{10^{-2}}{\mathcal{K}_T}\ \mathrm{T} \cdot \mathrm{m} = \frac{\mathcal{K}_A}{10^5}\ \mathrm{T} \cdot \mathrm{m} = 1.000000000274 \times 10^{-6}\ \mathrm{T} \cdot \mathrm{m}$.

When the vector potential depends on time we can calculate the electric field as in Eq. 3.69 and since $\frac{\bar{\mathrm{V}}_{\mathrm{cgs}}}{\bar{\mathrm{E}}_{\mathrm{cgs}} \cdot \bar{\mathrm{l}}_{\mathrm{cgs}}} = 1$ and $\frac{\bar{\mathrm{A}}_{\mathrm{cgs}}}{\bar{\mathrm{E}}_{\mathrm{cgs}} \cdot \bar{\mathrm{t}}_{\mathrm{cgs}}} = \frac{1}{\tilde{c}_{cgs}}$, in the c.g.s.-Gaussian system the electric field is given by:

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}. \tag{3.70}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{A}} = 1.24384033025 \times 10^{1}\ \mathrm{G} \cdot \mathrm{cm}$.

3.15 Magnetic field flux

In the SI the unit of the magnetic field flux (symbol Wb) is derived from its definition. The magnetic field flux through a surface perpendicular to $\hat{\mathbf{n}}$ is:

$$\Phi = \int \mathbf{B} \cdot \hat{\mathbf{n}}\, dS, \tag{3.71}$$

so the unit of the magnetic field flux is $\mathrm{Wb} = \mathrm{T} \cdot \mathrm{m}^2 = \frac{\mathrm{N \cdot s \cdot m}}{\mathrm{C}} = \mathrm{V} \cdot \mathrm{s} = \frac{\mathrm{N \cdot m}}{\mathrm{A}} = \frac{\mathrm{kg \cdot m^2}}{\mathrm{sC}} = \frac{\mathrm{J \cdot s}}{\mathrm{C}} = \frac{\mathrm{J}}{\mathrm{A}}$. This unit is called weber.

In a.u. the unit of the magnetic field flux (symbol $\bar{\mathrm{Wb}}$) can be derived from its definition $\bar{\mathrm{Wb}} = \bar{\mathrm{B}} \cdot \bar{\mathrm{l}}^2$. The conversion factor with the SI unit is:

$$\bar{\mathrm{Wb}} = \frac{\hbar}{e} = \frac{1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s}}{1.602176634 \times 10^{-19}\ \mathrm{C}} = 6.5821195695091 \times 10^{-16}\ \mathrm{Wb}. \tag{3.72}$$

In the c.g.s.-Gaussian system the unit of magnetic field flux (symbol Mx) is derived from its definition: $\mathrm{Mx} = \mathrm{G} \cdot \mathrm{cm}^2$. This unit is called maxwell. The conversion factor with the SI unit is:

$$\mathrm{Mx} = \frac{10^{-4}}{\mathcal{K}_T}\ \mathrm{T} \cdot \mathrm{m}^2 = 10^{-7}\ \mathcal{K}_A\ \mathrm{Wb} = 1.000000000274 \times 10^{-8}\ \mathrm{Wb} \tag{3.73}$$

In the old SI units this factor was 10^{-8}.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{Wb} = 6.58211956771 \times 10^{-8}\ \mathrm{Mx}$.

3.16 Inductance

In the SI the unit of the inductance (symbol H) is derived from its definition as the ratio of the magnetic field flux and the current in a circuit:

$$L = \frac{\Phi}{I}, \tag{3.74}$$

so the unit of inductance is $\mathrm{H} = \frac{\mathrm{Wb}}{\mathrm{A}} = \frac{\mathrm{T \cdot m^2}}{\mathrm{A}} = \frac{\mathrm{V \cdot s}}{\mathrm{A}} = \Omega \cdot \mathrm{s} = \frac{\mathrm{N \cdot m}}{\mathrm{A^2}} = \frac{\mathrm{J}}{\mathrm{A^2}} = \frac{\mathrm{kg \cdot m^2}}{\mathrm{C^2}}$. This unit is called henry.

In a.u. the unit of the inductance (symbol $\bar{\mathrm{Y}}$) can be derived from its definition as: $\bar{\mathrm{Y}} = \frac{\bar{\mathrm{Wb}}}{\bar{\mathrm{I}}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{Y}} = \frac{\hbar \bar{\mathrm{t}}}{e^2} = \frac{m_e a_B^2}{e^2} = \frac{\hbar^2}{E_h e^2} = \frac{(1.0545718176462 \times 10^{-34}\ \mathrm{J \cdot s})^2}{4.3597447222072 \times 10^{-18}\ \mathrm{J}\ (1.602176634 \times 10^{-19}\ \mathrm{C})^2} = 9.937347433815 \times 10^{-14}\ \mathrm{H}. \tag{3.75}$$

In the c.g.s.-Gaussian system the unit of inductance (symbol statH) is derived from its definition:

$$L = \frac{1}{c}\frac{\Phi}{I}. \tag{3.76}$$

This relationship shows that inductance has the dimensions of $\mathrm{s^2/cm}$. This unit is called stathenry. The conversion factor with the SI unit can be found by writing $\bar{\mathrm{Y}}_{\mathrm{cgs}} = \mathrm{statH}$ and

$$L = \frac{\bar{\Phi}_{\mathrm{cgs}}}{\bar{\mathrm{Y}}_{\mathrm{cgs}} \cdot \bar{\mathrm{I}}_{\mathrm{cgs}}} \frac{\Phi}{I}. \tag{3.77}$$

Comparing with Eq. 3.76 we obtain:

$$\bar{\mathrm{Y}}_{\mathrm{cgs}} = \frac{\tilde{c}_{cgs} \bar{\Phi}_{\mathrm{cgs}}}{\bar{\mathrm{I}}_{\mathrm{cgs}}}, \tag{3.78}$$

therefore:

$$\mathrm{statH} = \tilde{c}_{cgs} \frac{10^{-4}\mathcal{K}}{\mathcal{K}_T}\ \mathrm{H} = \tilde{c}_{cgs} 10^{-7} \mathcal{K}_A \mathcal{K}\ \mathrm{H} = 10^{-7}\mathcal{K}^2\ \mathrm{H} = 8.9875517923 \times 10^{11}\ \mathrm{H}. \tag{3.79}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{H}} = 1.10567901732 \times 10^{-25}\ \mathrm{statH}$.

3.17 Magnetic dipole moment

In the SI the unit of the magnetic dipole moment can be derived from its definition. For instance the magnetic dipole moment $\boldsymbol{\mu}$ of a coil traversed by a current I is:

$$\boldsymbol{\mu} = IA\hat{\mathbf{n}}, \tag{3.80}$$

where A is the area of the coil and $\hat{\mathbf{n}}$ is a versor normal to the area. Therefore the unit of the magnetic dipole moment is $\mathrm{A}\cdot\mathrm{m}^2 = \frac{\mathrm{N\cdot m\cdot A\cdot m}}{\mathrm{N}} = \mathrm{J/T}$.

In a.u. the unit of the magnetic dipole moment (symbol $\bar{\mu}$) is derived from its definition as $\bar{\mu} = \bar{\mathrm{I}}\cdot\bar{\mathrm{l}}^2$. The conversion factor with the SI unit is:

$$\begin{aligned}\bar{\mu} = \frac{\bar{\mathrm{C}}\cdot\bar{\mathrm{l}}^2}{\bar{\mathrm{t}}} = \frac{ea_B^2\hbar}{m_e a_B^2} = \frac{\hbar e}{m_e} = 2\mu_B &= \frac{1.0545718176462\times10^{-34}\ \mathrm{J\cdot s}\ 1.602176634\times10^{-19}\ \mathrm{C}}{9.1093837015\times10^{-31}\ \mathrm{kg}}\\ &= 1.85480201567\times10^{-23}\mathrm{J/T}.\end{aligned} \tag{3.81}$$

In the c.g.s.-Gaussian system the unit of magnetic dipole moment (symbol $\bar{\mu}_{\mathrm{cgs}}$) is derived from its definition:

$$\boldsymbol{\mu} = \frac{1}{c}IA\hat{\mathbf{n}}, \tag{3.82}$$

hence its dimensions are $\mathrm{statC}\cdot\mathrm{cm}$. To find the conversion factor with the SI unit we use Eq. 3.80 for a current I $\bar{\mathrm{I}}_{\mathrm{cgs}}$ and area A $\bar{\mathrm{l}}^2_{\mathrm{cgs}}$ that gives a dipole moment $\bar{\mu}_{\mathrm{cgs}}\boldsymbol{\mu}$. We have therefore:

$$\boldsymbol{\mu} = \frac{\bar{\mathrm{I}}_{\mathrm{cgs}}\cdot\bar{\mathrm{l}}^2_{\mathrm{cgs}}}{\bar{\mu}_{cgs}}IA\hat{\mathbf{n}}. \tag{3.83}$$

Comparing with Eq. 3.82 we obtain:

$$\bar{\mu}_{cgs} = \tilde{c}_{cgs}\bar{\mathrm{I}}_{\mathrm{cgs}}\cdot\bar{\mathrm{l}}^2_{\mathrm{cgs}} = \frac{\tilde{c}_{cgs}10^{-4}}{\mathcal{K}}\ \mathrm{A\cdot m^2} = \frac{1}{10^4\mathcal{K}_A}\ \mathrm{A\cdot m^2} = 9.99999999726\times10^{-4}\ \mathrm{A\cdot m^2}. \tag{3.84}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mu} = 1.85480201618\times10^{-20}\ \mathrm{statC\cdot cm}$.

3.18 Magnetization

In the SI the unit of the magnetization can be derived from its definition as the magnetic dipole moment per unit volume:

$$\mathrm{M} = \frac{\boldsymbol{\mu}}{V}, \tag{3.85}$$

where V is the volume of the sample. Therefore the unit of the magnetization is $\frac{\mathrm{A}}{\mathrm{m}}$.

In a.u. the unit of the magnetization (symbol $\bar{\mathrm{M}}$) is derived from its definition as $\bar{\mathrm{M}} = \frac{\bar{\mathrm{I}}}{\bar{\mathrm{l}}}$. The conversion factor with the SI unit is:

$$\bar{\mathrm{M}} = \frac{6.623618237510 \times 10^{-3}\ \mathrm{A}}{5.29177210903 \times 10^{-11}\ \mathrm{m}} = 1.25168244230 \times 10^{8} \mathrm{A/m}. \tag{3.86}$$

Using the expression of $\bar{\mu}$ and $\bar{\mathrm{l}}$ we can write also:

$$\bar{M} = \frac{2\mu_B}{a_B^3}. \tag{3.87}$$

In the c.g.s.-Gaussian system the unit of magnetization (symbol $\bar{\mathrm{M}}_{\mathrm{cgs}}$) is derived from its definition: $\bar{\mathrm{M}}_{\mathrm{cgs}} = \frac{\mathrm{statC}}{\mathrm{cm}^2}$. The conversion with the SI unit is:

$$\bar{\mathrm{M}}_{\mathrm{cgs}} = \frac{\bar{\mu}_{cgs}}{\mathrm{cm}^3} = \frac{1}{10^{-2}\ \mathcal{K}_A}\ \mathrm{A/m} = 9.99999999726 \times 10^{2}\ \mathrm{A/m}. \tag{3.88}$$

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{M}} = 1.25168244264 \times 10^{5}\ \mathrm{statC/cm}^2$.

3.19 Vacuum magnetic permeability

In the SI the unit of the vacuum magnetic permeability μ_0 be derived from the equation:

$$\mu_0 = \frac{1}{c^2 \epsilon_0}, \tag{3.89}$$

where c is the speed of light. Therefore the unit of μ_0 is $\frac{\mathrm{N \cdot s^2}}{\mathrm{C^2}} = \frac{\mathrm{N}}{\mathrm{A^2}} = \frac{\mathrm{V \cdot s}}{\mathrm{A \cdot m}} = \frac{\mathrm{H}}{\mathrm{m}} = \frac{\mathrm{m \cdot T}}{\mathrm{A}}$. Its numerical value is given in Eq. 1.11 and it is approximately $4\pi \times 10^{-7}$.

In a.u. the vacuum magnetic permeability μ_0 is not used.

In the c.g.s.-Gaussian system μ_0 is not used.

3.20 Magnetic field strength

In the SI the magnetic field strength is given in term of the magnetic flux density and of the magnetization by:

$$\mathbf{H} = \frac{\mathbf{B}}{\mu_0} - \mathbf{M}, \tag{3.90}$$

so the magnetic field and the magnetization have the same unit $\frac{\mathrm{A}}{\mathrm{m}}$. Eq. 3.90 can be derived from the fourth Maxwell's equation:

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}. \tag{3.91}$$

Separating $\mathbf{J} = \mathbf{J}_f + \mathbf{J}_m + \mathbf{J}_d$ where $\mathbf{J}_f$ is the current of the free charges,

$$\mathbf{J}_m = \nabla \times \mathbf{M} \tag{3.92}$$

is the magnetization current, and

$$\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t} \tag{3.93}$$

is the displacement current and inserting these expressions in Eq. 3.91 one obtains, after dividing by μ_0:

$$\nabla \times (\frac{\mathbf{B}}{\mu_0} - \mathbf{M}) = \mathbf{J}_f + \frac{\partial(\mathbf{P} + \epsilon_0 \mathbf{E})}{\partial t}. \tag{3.94}$$

Using Eq. 3.90 and the definition of D the fourth macroscopic Maxwell's equation becomes:

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}. \tag{3.95}$$

In a.u. the unit of magnetic field strength ($\bar{\mathrm{H}}$) can be derived from the relationship between magnetic field strength, magnetic flux density, and magnetization. This relationship can be derived writing Eq. 3.91 in a.u.. We have:

$$\nabla \times \mathbf{B} = \frac{\mu_0 \bar{\mathrm{J}} \cdot \bar{\mathrm{l}}}{\bar{\mathrm{B}}}\mathbf{J} + \frac{\bar{\mathrm{E}} \cdot \bar{\mathrm{l}}}{c^2 \bar{\mathrm{t}} \cdot \bar{\mathrm{B}}}\frac{\partial \mathbf{E}}{\partial t}. \tag{3.96}$$

Since $\frac{\mu_0 \bar{\mathrm{J}} \cdot \bar{\mathrm{l}}}{\bar{\mathrm{B}}} = 4\pi\alpha^2$ and $\frac{\bar{\mathrm{E}} \cdot \bar{\mathrm{l}}}{c^2 \bar{\mathrm{t}} \cdot \bar{\mathrm{B}}} = \alpha^2$, where α is the fine structure constant, this equation becomes:

$$\nabla \times \mathbf{B} = 4\pi\alpha^2 \mathbf{J} + \alpha^2 \frac{\partial \mathbf{E}}{\partial t}. \tag{3.97}$$

Moreover we have:

$$\mathbf{J}_m = \frac{\bar{\mathrm{M}}}{\bar{\mathrm{l}} \cdot \bar{\mathrm{J}}} \nabla \times \mathbf{M} \tag{3.98}$$

and

$$\mathbf{J}_d = \frac{\bar{\mathrm{P}}}{\bar{\mathrm{t}} \cdot \bar{\mathrm{J}}} \frac{\partial \mathbf{P}}{\partial t}. \tag{3.99}$$

Since $\frac{\bar{\mathrm{M}}}{\bar{\mathrm{l}} \cdot \bar{\mathrm{J}}} = 1$ and $\frac{\bar{\mathrm{P}}}{\bar{\mathrm{t}} \cdot \bar{\mathrm{J}}} = 1$ we have:

$$\mathbf{J}_m = \nabla \times \mathbf{M} \tag{3.100}$$

and

$$\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t}, \tag{3.101}$$

as in the SI. Therefore after division by α^2 Eq. 3.97 becomes:

$$\nabla \times (\frac{\mathbf{B}}{\alpha^2} - 4\pi \mathbf{M}) = 4\pi \mathbf{J}_f + \frac{\partial(\mathbf{E} + 4\pi \mathbf{P})}{\partial t}. \tag{3.102}$$

This equation suggests the definition of the magnetic field strength as:

$$\mathbf{H} = \frac{\mathbf{B}}{\alpha^2} - 4\pi \mathbf{M}, \tag{3.103}$$

that gives the macroscopic Maxwell's equation:

$$\nabla \times \mathbf{H} = 4\pi \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}. \tag{3.104}$$

Finally, we can find $\bar{\mathrm{H}}$ by writing:

$$\mathbf{H} = \frac{\bar{\mathrm{B}}}{\mu_0 \bar{\mathrm{H}}} \mathbf{B} - \frac{\bar{\mathrm{M}}}{\bar{\mathrm{H}}} \mathbf{M}. \tag{3.105}$$

Comparing with Eq. 3.103 we obtain:

$$\bar{\mathrm{H}} = \frac{\bar{\mathrm{B}} \alpha^2}{\mu_0} = \frac{\bar{\mathrm{M}}}{4\pi}. \tag{3.106}$$

Therefore the conversion factor with the SI unit is:

$$\bar{H} = 9.9605723936 \times 10^6 \ \mathrm{A/m}. \tag{3.107}$$

In the c.g.s.-Gaussian system the unit of the magnetic field strength (symbol Oe) is derived from the relationship between magnetic field strength, magnetic flux density, and magnetization. This relationship can be derived as discussed for the a.u. case. In Eq. 3.96 we have $\frac{\mu_0 \bar{\mathrm{J}}_{\mathrm{cgs}} \cdot \bar{\mathrm{l}}_{\mathrm{cgs}}}{\bar{\mathrm{B}}_{\mathrm{cgs}}} = \frac{4\pi}{c_{cgs}}$ and $\frac{\bar{\mathrm{E}}_{\mathrm{cgs}} \cdot \bar{\mathrm{l}}_{\mathrm{cgs}}}{c^2 \bar{\mathrm{t}}_{\mathrm{cgs}} \cdot \bar{\mathrm{B}}_{\mathrm{cgs}}} = \frac{1}{c_{cgs}}$ so the Maxwell's equation becomes:

$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t}. \tag{3.108}$$

Moreover we have: $\frac{\bar{\mathrm{M}}_{\mathrm{cgs}}}{\bar{\mathrm{l}}_{\mathrm{cgs}} \cdot \bar{\mathrm{J}}_{\mathrm{cgs}}} = \frac{\mathcal{K}}{\mathcal{K}_A} = c_{cgs}$ and $\frac{\bar{\mathrm{P}}_{\mathrm{cgs}}}{\bar{\mathrm{t}}_{\mathrm{cgs}} \cdot \bar{\mathrm{J}}_{\mathrm{cgs}}} = 1$ so in c.g.s. units:

$$\mathbf{J}_m = c\nabla \times \mathbf{M} \tag{3.109}$$

and

$$\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t}. \tag{3.110}$$

Inserting these expressions in the Maxwell's equation we have:

$$\nabla \times (\mathbf{B} - 4\pi\mathbf{M}) = \frac{4\pi}{c}\mathbf{J}_f + \frac{1}{c}\frac{\partial(\mathbf{E} + 4\pi\mathbf{P})}{\partial t}. \tag{3.111}$$

This equation suggests the definition of the magnetic field strength as:

$$\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}, \tag{3.112}$$

that gives the macroscopic Maxwell's equation:

$$\nabla \times \mathbf{H} = \frac{4\pi}{c}\mathbf{J}_f + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}. \tag{3.113}$$

Comparing Eq. 3.112 and Eq. 3.105, we can find the conversion factor with the SI unit. We have $\mathrm{Oe} = \frac{\bar{\mathrm{B}}_{\mathrm{cgs}}}{\mu_0} = \frac{\bar{\mathrm{M}}_{\mathrm{cgs}}}{4\pi}$ or

$$\mathrm{Oe} = \frac{1}{4\pi\ 10^{-2}\mathcal{K}_A}\mathrm{A/m} = 7.95774715242 \times 10^1\ \mathrm{A/m}. \tag{3.114}$$

This unit is called oersted.

The conversion factor between the a.u. and the c.g.s.-Gaussian unit is: $\bar{\mathrm{H}} = 1.25168244264 \times 10^5\ \mathrm{statC/cm^2}$.

3.21 Microscopic Maxwell's equations

In the SI the microscopic Maxwell's equations are:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{3.115}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{3.116}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{3.117}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}. \tag{3.118}$$

The form of the microscopic Maxwell's equations in a.u. has been obtained in the previous text:

$$\nabla \cdot \mathbf{E} = 4\pi\rho, \tag{3.119}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{3.120}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{3.121}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c^2}\mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}, \tag{3.122}$$

where in these equations c is actually $c_{a.u.} = \frac{1}{\alpha}$ and all other quantities are measured in a.u..

The form of the microscopic Maxwell's equations in the c.g.s-Gaussian system has been discussed in the previous text:

$$\nabla \cdot \mathbf{E} = 4\pi\rho, \tag{3.123}$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \tag{3.124}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{3.125}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t}, \tag{3.126}$$

where in these equations c is actually c_{cgs} and all other quantities are measured in c.g.s.-Gaussian units.

3.22 Macroscopic Maxwell's equations

In the SI the macroscopic Maxwell's equations can be formally obtained first by averaging the microscopic equations and then dividing the macroscopic charge density into a free part and a bound part $\rho = \rho_f + \rho_b$ with $\rho_b = -\nabla \cdot \mathbf{P}$ where $\mathbf{P}$ is the polarization. Similarly the macroscopic current density is divided into a free part, a magnetization part, and a displacement part with $\mathbf{J} = \mathbf{J}_f + \mathbf{J}_m + \mathbf{J}_d$ where $\mathbf{J}_m = \nabla \times \mathbf{M}$ and $\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t}$. Inserting these expressions we have:

$$\nabla \cdot \mathbf{D} = \rho_f, \tag{3.127}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{3.128}$$
$$\nabla \cdot \mathbf{B} = 0, \tag{3.129}$$
$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}. \tag{3.130}$$

where $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$ and $\mathbf{H} = \frac{\mathbf{B}}{\mu_0} - \mathbf{M}$.

The form of the macroscopic Maxwell's equations in a.u. has been discussed in the previous text. We can write $\rho = \rho_f + \rho_b$ with $\rho_b = -\nabla \cdot \mathbf{P}$ where $\mathbf{P}$ is the polarization. Similarly the current density can be divided into a free part, a magnetization part, and a displacement part with $\mathbf{J} = \mathbf{J}_f + \mathbf{J}_m + \mathbf{J}_d$ where $\mathbf{J}_m = \nabla \times \mathbf{M}$ and $\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t}$ We have:

$$\nabla \cdot \mathbf{D} = 4\pi \rho_f, \tag{3.131}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{3.132}$$
$$\nabla \cdot \mathbf{B} = 0, \tag{3.133}$$
$$\nabla \times \mathbf{H} = 4\pi \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}. \tag{3.134}$$

where $\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P}$ and $\mathbf{H} = c^2 \mathbf{B} - 4\pi \mathbf{M}$. Here c is $c_{a.u.} = \frac{1}{\alpha}$ and all other quantities are measured in a.u..

The form of the macroscopic Maxwell's equations in the c.g.s-Gaussian system has been discussed in the previous text. In these units $\rho = \rho_f + \rho_b$ with $\rho_b = -\nabla \cdot \mathbf{P}$ where $\mathbf{P}$ is the polarization. Similarly the current density can be divided into a free part, a magnetization part, and a displacement part with

$\mathbf{J} = \mathbf{J}_f + \mathbf{J}_m + \mathbf{J}_d$ where $\mathbf{J}_m = c\nabla \times \mathbf{M}$ and $\mathbf{J}_d = \frac{\partial \mathbf{P}}{\partial t}$

$$\nabla \cdot \mathbf{D} = 4\pi\rho_f, \tag{3.135}$$

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \tag{3.136}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{3.137}$$

$$\nabla \times \mathbf{H} = \frac{4\pi}{c}\mathbf{J}_f + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}, \tag{3.138}$$

where $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$ and $\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}$. In these equations c is actually c_{cgs} and all other quantities are measured in c.g.s.-Gaussian units.

Chapter 4

Quantum Mechanics

4.1 The Schrödinger equation

In the SI the time independent Schrödinger equation for a particle with charge q, mass m and spin $1/2$ in an electromagnetic field described by the scalar potential $\phi(\mathbf{r})$ and the vector potential $\mathbf{A}(\mathbf{r})$ is:

$$\left[\frac{1}{2m}(\mathbf{p}-q\mathbf{A})^2+q\phi-\frac{q\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}) \tag{4.1}$$

where $\mathbf{B}=\nabla\times\mathbf{A}$, $\boldsymbol{\sigma}$ are the Pauli matrices and $\Psi(\mathbf{r})$ is a two component spinor.

In a.u. the time independent Schrödinger equation becomes:

$$\left[\frac{1}{2m\bar{\mathrm{m}}}(\bar{\mathrm{p}}\mathbf{p}-\bar{\mathrm{C}}\cdot\bar{\mathrm{A}}q\mathbf{A})^2+\bar{\mathrm{C}}\cdot\bar{\mathrm{V}}q\phi-\frac{\bar{\mathrm{C}}\cdot\bar{\mathrm{B}}}{\bar{\mathrm{m}}}\frac{\hbar q}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r})=\bar{\mathrm{E}}E\Psi(\mathbf{r}) \tag{4.2}$$

Using $\bar{\mathrm{p}}=\frac{\hbar}{a_B}$, $\bar{\mathrm{A}}=\frac{\hbar}{ea_B}$, $\bar{\mathrm{C}}=e$, $\bar{\mathrm{V}}=\frac{E_h}{e}$, $\bar{\mathrm{B}}=\frac{\hbar}{ea_B^2}$ and $\bar{\mathrm{E}}=E_h$ we get

$$\left[\frac{\hbar^2}{m_ea_B^2}\frac{1}{2m}(\mathbf{p}-q\mathbf{A})^2+E_hq\phi-\frac{\hbar^2}{m_ea_B^2}\frac{q}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r})=E_hE\Psi(\mathbf{r}) \tag{4.3}$$

but since $E_h=\frac{\hbar^2}{m_ea_B^2}$ the equation can be simplified into

$$\left[\frac{1}{2m}(\mathbf{p}-q\mathbf{A})^2+q\phi-\frac{q}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}) \tag{4.4}$$

where all quantities are in a.u..

For an electron $m=1$ and $q=-1$ and one should write:

$$\left[\frac{1}{2}(\mathbf{p}+\mathbf{A})^2-\phi+\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}). \tag{4.5}$$

However this form is rarely used. One prefers to introduce the potential energy of the electron $V = q\phi$ and keep the symbol $\mu_B = -\frac{1}{2}$ so that the equation is written:

$$\left[\frac{1}{2}(\mathbf{p}+\mathbf{A})^2 + V - \mu_B \boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{4.6}$$

When $\mathbf{A} = 0$ we can write explicitly $\mathbf{p} = -i\nabla$, and the Schrödinger equation becomes:

$$\left[-\frac{1}{2}\nabla^2 + V - \mu_B \boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{4.7}$$

The form of the Schrödinger equation in the c.g.s.-Gaussian system can be found starting from Eq. 4.2 and using: $\bar{\mathrm{p}}_{\mathrm{cgs}} = 10^{-5}\frac{\mathrm{kg\cdot m}}{\mathrm{s}}$, $\bar{\mathrm{C}}_{\mathrm{cgs}}\cdot\bar{\mathrm{A}}_{\mathrm{cgs}} = \frac{1}{\mathcal{K}}\frac{10^{-2}}{\mathcal{K}_T}\ \mathrm{C\cdot T\cdot m} = \frac{10^{-5}}{\tilde{c}_{cgs}}\frac{\mathrm{kg\cdot m}}{\mathrm{s}}$, $\bar{\mathrm{C}}_{\mathrm{cgs}}\cdot\bar{\mathrm{V}}_{\mathrm{cgs}} = \frac{1}{\mathcal{K}}10^{-7}\mathcal{K}\ \mathrm{C\cdot V} = 10^{-7}\mathrm{J}$, $\frac{\bar{\mathrm{C}}_{\mathrm{cgs}}\cdot\bar{\mathrm{B}}_{\mathrm{cgs}}\hbar}{\bar{\mathrm{m}}_{\mathrm{cgs}}} = \tilde{\hbar}\frac{1}{\mathcal{K}}\frac{1}{\mathcal{K}_T 10^{-3}}\mathrm{J} = \frac{10^{-7}\tilde{\hbar}_{cgs}}{\tilde{c}_{cgs}}\mathrm{J}$, and $\bar{\mathrm{E}}_{\mathrm{cgs}} = 10^{-7}\mathrm{J}$ leading to:

$$\left[\frac{1}{2m}(\mathbf{p}-\frac{q}{c}\mathbf{A})^2 + q\phi - \frac{\hbar q}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{4.8}$$

where all quantities are expressed in c.g.s.-Gaussian units.

Appendix A

Rydberg atomic units

In this Appendix we discuss the Rydberg a.u. using the same symbols used for Hartree a.u. with the subscript R. Rydberg a.u. are defined requiring that $a_B = \bar{\mathrm{l}}_\mathrm{R}$, $m_e = \frac{1}{2}\,\bar{\mathrm{m}}_\mathrm{R}$, $e = \sqrt{2}\,\bar{\mathrm{C}}_\mathrm{R}$ and $\hbar = \frac{\bar{\mathrm{m}}_\mathrm{R}\cdot\bar{\mathrm{l}}_\mathrm{R}^2}{\bar{\mathrm{t}}_\mathrm{R}}$. We have therefore

$$\bar{\mathrm{l}}_\mathrm{R} = a_B = \bar{\mathrm{l}}, \tag{A.1}$$

$$\bar{\mathrm{m}}_\mathrm{R} = 2m_e = 2\bar{\mathrm{m}} = 1.82187674030 \times 10^{-30}\ \mathrm{kg}, \tag{A.2}$$

$$\bar{\mathrm{C}}_\mathrm{R} = \frac{e}{\sqrt{2}} = \frac{\bar{\mathrm{C}}}{\sqrt{2}} = 1.1329099625600 \times 10^{-19}\ \mathrm{C}, \tag{A.3}$$

$$\bar{\mathrm{t}}_\mathrm{R} = \frac{\bar{\mathrm{m}}_\mathrm{R}\cdot\bar{\mathrm{l}}_\mathrm{R}^2}{\hbar} = \frac{2m_e a_B^2}{\hbar} = 2\bar{\mathrm{t}} = 4.8377686531714 \times 10^{-17}\ \mathrm{s}. \tag{A.4}$$

Using these relationships we can derive the conversion factors for the other units discussed in the text.

Frequency:

$$\bar{\nu}_R = \frac{1}{\bar{\mathrm{t}}_\mathrm{R}} = \frac{1}{2\bar{\mathrm{t}}} = \frac{1}{2}\bar{\nu} = 2.0670686667591 \times 10^{16}\ \mathrm{Hz}. \tag{A.5}$$

Speed:

$$\bar{\mathrm{v}}_\mathrm{R} = \frac{\bar{\mathrm{l}}_\mathrm{R}}{\bar{\mathrm{t}}_\mathrm{R}} = \frac{\bar{\mathrm{l}}}{2\bar{\mathrm{t}}} = \frac{1}{2}\bar{\mathrm{v}} = 1.09384563182 \times 10^{6}\ \mathrm{m/s}. \tag{A.6}$$

Acceleration:

$$\bar{\mathrm{a}}_\mathrm{R} = \frac{\bar{\mathrm{l}}_\mathrm{R}}{\bar{\mathrm{t}}_\mathrm{R}^2} = \frac{\bar{\mathrm{l}}}{4\bar{\mathrm{t}}^2} = \frac{1}{4}\bar{\mathrm{a}} = 4.52210806362 \times 10^{22}\ \mathrm{m/s^2}. \tag{A.7}$$

Momentum:

$$\bar{\mathrm{p}}_\mathrm{R} = \frac{\bar{\mathrm{m}}_\mathrm{R}\cdot\bar{\mathrm{l}}_\mathrm{R}}{\bar{\mathrm{t}}_\mathrm{R}} = \frac{2\bar{\mathrm{m}}\cdot\bar{\mathrm{l}}}{2\bar{\mathrm{t}}} = \bar{\mathrm{p}}. \tag{A.8}$$

Angular momentum:

$$\bar{\mathrm{L}}_\mathrm{R} = \frac{\bar{\mathrm{m}}_\mathrm{R}\cdot\bar{\mathrm{l}}_\mathrm{R}^2}{\bar{\mathrm{t}}_\mathrm{R}} = \frac{2\bar{\mathrm{m}}\cdot\bar{\mathrm{l}}^2}{2\bar{\mathrm{t}}} = \bar{\mathrm{L}}. \tag{A.9}$$

Force:

$$\bar{\mathrm{f}}_\mathrm{R} = \frac{\bar{\mathrm{m}}_\mathrm{R}\cdot\bar{\mathrm{l}}_\mathrm{R}}{\bar{\mathrm{t}}_\mathrm{R}^2} = \frac{2\bar{\mathrm{m}}\cdot\bar{\mathrm{l}}}{4\bar{\mathrm{t}}^2} = \frac{1}{2}\bar{\mathrm{f}} = 4.11936174912 \times 10^{-8}\ \mathrm{N}. \tag{A.10}$$

Energy:

$$\bar{\mathrm{U}}_{\mathrm{R}} = \bar{\mathrm{f}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}} = \frac{1}{2}\bar{\mathrm{f}} \cdot \bar{\mathrm{l}} = \frac{1}{2}\bar{\mathrm{U}} = 2.1798723611036 \times 10^{-18}\ \mathrm{J}. \tag{A.11}$$

Power:

$$\bar{\mathrm{W}}_{\mathrm{R}} = \frac{\bar{\mathrm{U}}_{\mathrm{R}}}{\bar{\mathrm{t}}_{\mathrm{R}}} = \frac{\bar{\mathrm{U}}}{4\bar{\mathrm{t}}} = \frac{1}{4}\bar{\mathrm{W}} = 4.505945855171 \times 10^{-2}\ \mathrm{W}. \tag{A.12}$$

Pressure:

$$\bar{\sigma}_{\mathrm{R}} = \frac{\bar{\mathrm{f}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}^2} = \frac{\bar{\mathrm{U}}}{2\bar{\mathrm{l}}^2} = \frac{1}{2}\bar{\sigma} = 1.47105078482 \times 10^{13}\ \mathrm{Pa}. \tag{A.13}$$

Current:

$$\bar{\mathrm{I}}_{\mathrm{R}} = \frac{\bar{\mathrm{C}}_{\mathrm{R}}}{\bar{\mathrm{t}}_{\mathrm{R}}} = \frac{\bar{\mathrm{C}}}{2\sqrt{2}\ \bar{\mathrm{t}}} = \frac{1}{2\sqrt{2}}\bar{\mathrm{I}} = 2.3418026858671 \times 10^{-3}\ \mathrm{A}. \tag{A.14}$$

Charge density:

$$\bar{\rho}_{\mathrm{R}} = \frac{\bar{\mathrm{C}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}^3} = \frac{\bar{\mathrm{C}}}{\sqrt{2}\ \bar{\mathrm{l}}^3} = \frac{1}{\sqrt{2}}\bar{\rho} = 7.6452553796 \times 10^{11}\ \mathrm{C/m^3}. \tag{A.15}$$

Current density:

$$\bar{\mathrm{J}}_{\mathrm{R}} = \frac{\bar{\mathrm{I}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}^2} = \frac{\bar{\mathrm{I}}}{2\sqrt{2}\ \bar{\mathrm{l}}^2} = \frac{1}{2\sqrt{2}}\bar{\mathrm{J}} = 8.36272920114 \times 10^{17}\ \mathrm{A/m^2}. \tag{A.16}$$

Electric field:

$$\bar{\mathrm{E}}_{\mathrm{R}} = \frac{\bar{\mathrm{f}}_{\mathrm{R}}}{\bar{\mathrm{C}}_{\mathrm{R}}} = \frac{\sqrt{2}\ \bar{\mathrm{f}}}{2\bar{\mathrm{C}}} = \frac{1}{\sqrt{2}}\bar{\mathrm{E}} = 3.63608926151 \times 10^{11}\ \mathrm{N/C}. \tag{A.17}$$

Electric potential:

$$\bar{\mathrm{V}}_{\mathrm{R}} = \bar{\mathrm{E}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}} = \frac{\bar{\mathrm{E}}}{\sqrt{2}\ \bar{\mathrm{l}}} = \frac{1}{\sqrt{2}}\bar{\mathrm{V}} = 1.9241355740025 \times 10^{1}\ \mathrm{V}. \tag{A.18}$$

Capacitance:

$$\bar{\mathrm{F}}_{\mathrm{R}} = \frac{\bar{\mathrm{C}}_{\mathrm{R}}}{\bar{\mathrm{V}}_{\mathrm{R}}} = \frac{\sqrt{2}\ \bar{\mathrm{C}}}{\sqrt{2}\ \bar{\mathrm{V}}} = \bar{\mathrm{F}}. \tag{A.19}$$

Electric dipole moment:

$$\bar{\wp}_{\mathrm{R}} = \bar{\mathrm{C}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}} = \frac{1}{\sqrt{2}}\bar{\mathrm{C}} \cdot \bar{\mathrm{l}} = \frac{1}{\sqrt{2}}\bar{\wp} = 5.99510134192 \times 10^{-30}\ \mathrm{C \cdot m}. \tag{A.20}$$

Polarization:

$$\bar{\mathrm{P}}_{\mathrm{R}} = \frac{\bar{\mathrm{C}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}^2} = \frac{\bar{\mathrm{C}}}{\sqrt{2}\ \bar{\mathrm{l}}^2} = \frac{1}{\sqrt{2}}\bar{\mathrm{P}} = 4.0456949184 \times 10^{1}\ \mathrm{C/m^2}. \tag{A.21}$$

Resistence:

$$\bar{\Omega}_{R} = \frac{\bar{\mathrm{V}}_{\mathrm{R}}}{\bar{\mathrm{I}}_{\mathrm{R}}} = \frac{2\sqrt{2}\ \bar{\mathrm{V}}}{\sqrt{2}\ \bar{\mathrm{I}}} = 2\bar{\Omega} = 8.2164718044553 \times 10^{3}\ \Omega. \tag{A.22}$$

Magnetic flux density:

$$\bar{\mathrm{B}}_{\mathrm{R}} = \frac{\bar{\mathrm{f}}_{\mathrm{R}}}{\bar{\mathrm{C}}_{\mathrm{R}} \cdot \bar{\mathrm{v}}_{\mathrm{R}}} = \frac{2\sqrt{2}\,\bar{\mathrm{f}}}{2\bar{\mathrm{C}} \cdot \bar{\mathrm{v}}} = \sqrt{2}\bar{\mathrm{B}} = 3.3241338227 \times 10^{5}\ \mathrm{T}. \tag{A.23}$$

Vector potential:

$$\bar{\mathrm{A}}_{\mathrm{R}} = \bar{\mathrm{B}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}} = \sqrt{2}\ \bar{\mathrm{B}} \cdot \bar{\mathrm{l}} = \sqrt{2}\ \bar{\mathrm{A}} = 1.75905586495 \times 10^{-5}\ \mathrm{T} \cdot \mathrm{m}. \tag{A.24}$$

Magnetic field flux:

$$\bar{\mathrm{Wb}}_{\mathrm{R}} = \bar{\mathrm{B}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}}^{2} = \sqrt{2}\ \bar{\mathrm{B}} \cdot \bar{\mathrm{l}}^{2} = \sqrt{2}\ \bar{\mathrm{Wb}} = 9.3085227643611 \times 10^{-16}\ \mathrm{Wb}. \tag{A.25}$$

With this definition the Lorentz force remains:

$$\mathbf{F} = q\mathbf{E} + q\left(\mathbf{v} \times \mathbf{B}\right), \tag{A.26}$$

and since $\frac{\bar{\mathrm{l}}_{\mathrm{R}} \cdot \bar{\mathrm{B}}_{\mathrm{R}}}{\bar{\mathrm{E}}_{\mathrm{R}} \cdot \bar{\mathrm{t}}_{\mathrm{R}}} = \frac{\bar{\mathrm{l}}_{\mathrm{R}} \cdot \bar{\mathrm{B}}_{\mathrm{R}}}{\bar{\mathrm{E}}_{\mathrm{R}} \cdot \bar{\mathrm{t}}_{\mathrm{R}}} = 1$ the second Maxwell's equation remains:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{A.27}$$

Inductance:

$$\bar{\mathrm{Y}}_{\mathrm{R}} = \frac{\bar{\mathrm{Wb}}_{\mathrm{R}}}{\bar{\mathrm{I}}_{\mathrm{R}}} = 2(\sqrt{2})^{2}\ \frac{\bar{\mathrm{Wb}}}{\bar{\mathrm{I}}} = 4\bar{\mathrm{Y}} = 3.9749389735260 \times 10^{-13}\ \mathrm{H}. \tag{A.28}$$

Magnetic dipole moment:

$$\bar{\mu}_{\mathrm{R}} = \bar{\mathrm{I}}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}}^{2} = \frac{1}{2\sqrt{2}}\ \bar{\mathrm{I}} \cdot \bar{\mathrm{l}}^{2} = \frac{1}{2\sqrt{2}}\bar{\mu} = 6.5577154152 \times 10^{-24}\ \mathrm{A} \cdot \mathrm{m}^{2}. \tag{A.29}$$

Magnetization:

$$\bar{\mathrm{M}}_{\mathrm{R}} = \frac{\bar{\mathrm{I}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}} = \frac{1}{2\sqrt{2}}\bar{\mathrm{I}} \cdot \bar{\mathrm{l}} = \frac{1}{2\sqrt{2}}\bar{\mathrm{M}} = 4.42536571420 \times 10^{7}\ \mathrm{A/m}. \tag{A.30}$$

In order to discuss the units of the electric displacement and of the magnetic field strength, we need to discuss the Maxwell's equations. The first Maxwell's equation is

$$\nabla \cdot \mathbf{E} = 4\pi\rho, \tag{A.31}$$

since $\frac{\bar{\rho}_{\mathrm{R}} \cdot \bar{\mathrm{l}}_{\mathrm{R}}}{\epsilon_0 \bar{\mathrm{E}}_{\mathrm{R}}} = \frac{\bar{\rho} \cdot \bar{\mathrm{l}}}{\epsilon_0 \bar{\mathrm{E}}} = 4\pi$. Moreover since $\frac{\bar{\mathrm{P}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}} \cdot \bar{\rho}_{\mathrm{R}}} = \frac{\bar{\mathrm{P}}}{\bar{\mathrm{l}} \cdot \bar{\rho}} = 1$ in these units

$$\rho_b = -\nabla \cdot \mathbf{P}, \tag{A.32}$$

and the macroscopic Maxwell's equation becomes:

$$\nabla \cdot \left(\mathbf{E} + 4\pi\mathbf{P}\right) = 4\pi\rho_f, \tag{A.33}$$

suggesting the definition:

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}. \tag{A.34}$$

Therefore:

$$\bar{\mathrm{D}}_{\mathrm{R}} = \frac{\bar{\mathrm{P}}_{\mathrm{R}}}{4\pi} = \frac{1}{\sqrt{2}}\bar{\mathrm{D}} = 3.21946172254\ \mathrm{C/m^2}. \tag{A.35}$$

The fourth Maxwell's equation can be written using $\frac{\mu_0 \bar{\mathrm{J}}_{\mathrm{R}}\cdot\bar{\mathrm{l}}_{\mathrm{R}}}{\bar{\mathrm{B}}_{\mathrm{R}}} = \frac{1}{4}\frac{\mu_0\bar{\mathrm{J}}\cdot\bar{\mathrm{l}}}{\bar{\mathrm{B}}} = \pi\alpha^2$ and $\frac{\bar{\mathrm{E}}_{\mathrm{R}}\cdot\bar{\mathrm{l}}_{\mathrm{R}}}{c^2\bar{\mathrm{t}}_{\mathrm{R}}\cdot\bar{\mathrm{B}}_{\mathrm{R}}} = \frac{1}{4}\frac{\bar{\mathrm{E}}\cdot\bar{\mathrm{l}}}{c^2\bar{\mathrm{t}}\cdot\bar{\mathrm{B}}} = \frac{\alpha^2}{4}$ so we have:

$$\nabla\times\mathbf{B} = \pi\alpha^2\mathbf{J} + \frac{\alpha^2}{4}\frac{\partial\mathbf{E}}{\partial t}. \tag{A.36}$$

Since $\frac{\bar{\mathrm{M}}_{\mathrm{R}}}{\bar{\mathrm{l}}_{\mathrm{R}}\cdot\bar{\mathrm{J}}_{\mathrm{R}}} = \frac{\bar{\mathrm{M}}}{\bar{\mathrm{l}}\cdot\bar{\mathrm{J}}} = 1$ and $\frac{\bar{\mathrm{P}}_{\mathrm{R}}}{\bar{\mathrm{t}}_{\mathrm{R}}\cdot\bar{\mathrm{J}}_{\mathrm{R}}} = \frac{\bar{\mathrm{P}}}{\bar{\mathrm{t}}\cdot\bar{\mathrm{J}}} = 1$ we can write

$$\mathbf{J}_m = \nabla\times\mathbf{M} \tag{A.37}$$

and

$$\mathbf{J}_d = \frac{\partial\mathbf{P}}{\partial t}, \tag{A.38}$$

obtaining the equation

$$\nabla\times(\frac{4\mathbf{B}}{\alpha^2} - 4\pi\mathbf{M}) = 4\pi\mathbf{J}_f + \frac{\partial(\mathbf{E}+4\pi\mathbf{P})}{\partial t}. \tag{A.39}$$

Defining the magnetic field strengh as:

$$\mathbf{H} = \frac{4\mathbf{B}}{\alpha^2} - 4\pi\mathbf{M}, \tag{A.40}$$

we can write the fourth macroscopic Maxwell's equation as:

$$\nabla\times\mathbf{H} = 4\pi\mathbf{J}_f + \frac{\partial\mathbf{D}}{\partial t}. \tag{A.41}$$

Therefore we have:

$$\bar{\mathrm{H}}_{\mathrm{R}} = \frac{\bar{\mathrm{M}}_{\mathrm{R}}}{4\pi} = \frac{1}{\sqrt{2}}\frac{\bar{\mathrm{M}}}{4\pi} = \frac{1}{\sqrt{2}}\bar{\mathrm{H}} = 3.52159414202\times10^6\ \mathrm{A/m}. \tag{A.42}$$

We note also that $\frac{\bar{\mathrm{l}}_{\mathrm{R}}\cdot\bar{\mathrm{B}}_{\mathrm{R}}}{\bar{\mathrm{E}}_{\mathrm{R}}\cdot\bar{\mathrm{t}}_{\mathrm{R}}} = \frac{\bar{\mathrm{l}}\cdot\bar{\mathrm{B}}}{\bar{\mathrm{E}}\cdot\bar{\mathrm{t}}} = 1$ so the second Maxwell's equation remains:

$$\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t}. \tag{A.43}$$

Finally we consider the continuity equation. Since $\frac{\bar{\mathrm{t}}_{\mathrm{R}}\cdot\bar{\mathrm{J}}_{\mathrm{R}}}{\bar{\rho}_{\mathrm{R}}\cdot\bar{\mathrm{l}}_{\mathrm{R}}} = \frac{\bar{\mathrm{t}}\cdot\bar{\mathrm{J}}}{\bar{\rho}\cdot\bar{\mathrm{l}}} = 1$ this equation remains:

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot\mathbf{J}. \tag{A.44}$$

The form of the Schrödinger equation in Rydberg a.u. can be found starting from Eq. 4.2 and using: $\bar{\mathrm{p}}_{\mathrm{R}} = \bar{\mathrm{p}}$, $\bar{\mathrm{C}}_{\mathrm{R}}\cdot\bar{\mathrm{A}}_{\mathrm{R}} = \bar{\mathrm{C}}\cdot\bar{\mathrm{A}}$, $\bar{\mathrm{C}}_{\mathrm{R}}\cdot\bar{\mathrm{V}}_{\mathrm{R}} = \frac{1}{2}\bar{\mathrm{C}}\cdot\bar{\mathrm{V}}$, $\frac{\bar{\mathrm{C}}_{\mathrm{R}}\hbar\bar{\mathrm{B}}_{\mathrm{R}}}{\bar{\mathrm{m}}_{\mathrm{R}}} = \frac{1}{2}\frac{\bar{\mathrm{C}}\hbar\bar{\mathrm{B}}}{\bar{\mathrm{m}}}$, and $\bar{\mathrm{E}}_{\mathrm{R}} = \frac{1}{2}\bar{\mathrm{E}}$ leading to:

$$\left[\frac{1}{2m}(\mathbf{p}-q\mathbf{A})^2 + q\phi - \frac{q}{2m}\boldsymbol{\sigma}\cdot\mathbf{B}\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{A.45}$$

where all quantities are expressed in Rydberg a.u..

For an electron $m = \frac{1}{2}$ and $q = -\sqrt{2}$ and one should write:

$$\left[(\mathbf{p} + \sqrt{2}\mathbf{A})^2 - \sqrt{2}\phi + \sqrt{2}\boldsymbol{\sigma} \cdot \mathbf{B}\right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{A.46}$$

However this form is rarely used. One prefers to introduce the potential energy of the electron $V = q\phi$ and keep the symbol $\mu_B = \frac{q}{2m} = -\sqrt{2}$ so that the equation is written:

$$\left[(\mathbf{p} + \sqrt{2}\mathbf{A})^2 + V - \mu_B\boldsymbol{\sigma} \cdot \mathbf{B}\right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{A.47}$$

When $\mathbf{A} = 0$ we can write explicitly $\mathbf{p} = -i\nabla$, and the Schrödinger equation becomes:

$$\left[-\nabla^2 + V - \mu_B\boldsymbol{\sigma} \cdot \mathbf{B}\right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{A.48}$$

Appendix B

Gaussian atomic units

It is possible to make the electromagnetic equations in a.u. look like those of the c.g.s.-Gaussian system. This requires the modification of the units of the magnetic flux density, vector potential, magnetic field flux, magnetic dipole moment, magnetization, and magnetic field strength, while the other units remain unchanged. We discuss these quantities here using a subscript G to identify the modified units. Although the unit of inductance is not modified we discuss it since it depends on the definition of the magnetic field flux. In order to avoid confusion we use α which is the same in all systems, but these equations are sometimes written using the speed of light $c = \frac{1}{\alpha}$ instead of α.

Magnetic flux density:
The definition of the Lorentz force in these units should be:

$$\mathbf{F} = \alpha q(\mathbf{v} \times \mathbf{B}). \tag{B.1}$$

Therefore we must have $\frac{\bar{\mathrm{C}}_{\mathrm{G}} \cdot \bar{\mathrm{v}}_{\mathrm{G}} \cdot \bar{\mathrm{B}}_{\mathrm{G}}}{\bar{\mathrm{f}}_{\mathrm{G}}} = \alpha$. Since one takes $\bar{\mathrm{C}}_{\mathrm{G}} = \bar{\mathrm{C}}$, $\bar{\mathrm{v}}_{\mathrm{G}} = \bar{\mathrm{v}}$ and $\bar{\mathrm{f}}_{\mathrm{G}} = \bar{\mathrm{f}}$, we have

$$\bar{\mathrm{B}}_{\mathrm{G}} = \alpha \frac{\hbar}{e a_B^2} = \alpha \bar{\mathrm{B}} = 1.71525554109 \times 10^3\ \mathrm{T}. \tag{B.2}$$

With this conversion factor we have $\frac{\bar{\mathrm{l}}_{\mathrm{G}} \cdot \bar{\mathrm{B}}_{\mathrm{G}}}{\bar{\mathrm{E}}_{\mathrm{G}} \cdot \bar{\mathrm{t}}_{\mathrm{G}}} = \alpha \frac{\bar{\mathrm{l}} \cdot \bar{\mathrm{B}}}{\bar{\mathrm{E}} \cdot \bar{\mathrm{t}}} = \alpha$ and the second Maxwell's equation becomes:

$$\nabla \times \mathbf{E} = -\alpha \frac{\partial \mathbf{B}}{\partial t}. \tag{B.3}$$

Vector potential:
We still have $\mathbf{B} = \nabla \times \mathbf{A}$, therefore:

$$\bar{\mathrm{A}}_{\mathrm{G}} = \bar{\mathrm{B}}_{\mathrm{G}} \cdot \bar{\mathrm{l}}_{\mathrm{G}} = \alpha \bar{\mathrm{A}} = 9.0767414322 \times 10^{-8}\ \mathrm{T} \cdot \mathrm{m} \tag{B.4}$$

When the vector potential is time dependent it gives rise to an electric field given by:

$$\mathbf{E} = -\nabla \Phi - \alpha \frac{\partial \mathbf{A}}{\partial t} \tag{B.5}$$

since $\frac{\bar{\mathrm{A}}_\mathrm{G}}{\bar{\mathrm{t}}_\mathrm{G}\cdot\bar{\mathrm{E}}_\mathrm{G}} = \alpha\frac{\bar{\mathrm{A}}}{\bar{\mathrm{t}}\cdot\bar{\mathrm{E}}} = \alpha$.

Magnetic field flux:
We still have:

$$\bar{\Phi}_\mathrm{G} = \bar{\mathrm{B}}_\mathrm{G}\cdot\bar{\mathrm{l}}_\mathrm{G}^2 = \alpha\bar{\Phi} = 4.80320471520\times 10^{-18}\ \mathrm{Wb}. \tag{B.6}$$

Inductance:
To have the same equation as in the c.g.s.-Gaussian system:

$$L = \alpha\frac{\Phi}{I}, \tag{B.7}$$

we must have $\frac{\bar{\Phi}_\mathrm{G}}{\bar{\mathrm{I}}_\mathrm{G}\cdot\bar{\mathrm{Y}}_\mathrm{G}} = \alpha$ or:

$$\bar{\mathrm{Y}}_\mathrm{G} = \frac{\bar{\Phi}_\mathrm{G}}{\alpha\bar{\mathrm{I}}_\mathrm{G}} = \bar{\mathrm{Y}}. \tag{B.8}$$

Magnetic dipole moment:
To have the same equation as in the c.g.s.-Gaussian system:

$$\boldsymbol{\mu} = \alpha I A\hat{\mathbf{n}}, \tag{B.9}$$

we must have $\frac{\bar{\mathrm{I}}_\mathrm{G}\cdot\bar{\mathrm{l}}_\mathrm{G}^2}{\bar{\mu}_\mathrm{G}} = \alpha$ or

$$\bar{\mu}_\mathrm{G} = \frac{\bar{\mathrm{I}}_\mathrm{G}\cdot\bar{\mathrm{l}}_\mathrm{G}^2}{\alpha} = \frac{1}{\alpha}\bar{\mu} = 2.5417464732\times 10^{-21}\ \mathrm{A}\cdot\mathrm{m}^2. \tag{B.10}$$

Magnetization:
We still have:

$$\bar{\mathrm{M}}_\mathrm{G} = \frac{\bar{\mu}_\mathrm{G}}{\bar{\mathrm{l}}_\mathrm{G}^3} = \frac{1}{\alpha}\bar{\mathrm{M}} = 1.71525554016\times 10^{10}\ \mathrm{A/m}. \tag{B.11}$$

Magnetic field strength:
The unit of the magnetic field strength is derived from the relationship between magnetic field flux, magnetization, and magnetic field strength. Since $\frac{\mu_0\bar{\mathrm{J}}_\mathrm{G}\cdot\bar{\mathrm{l}}_\mathrm{G}}{\bar{\mathrm{B}}_\mathrm{G}} = \frac{\mu_0\bar{\mathrm{J}}\cdot\bar{\mathrm{l}}}{\alpha\bar{\mathrm{B}}} = 4\pi\alpha$ and $\frac{\bar{\mathrm{E}}_\mathrm{G}\cdot\bar{\mathrm{l}}_\mathrm{G}}{c^2\bar{\mathrm{t}}_\mathrm{G}\cdot\bar{\mathrm{B}}_\mathrm{G}} = \frac{\bar{\mathrm{E}}\cdot\bar{\mathrm{l}}}{c^2\bar{\mathrm{t}}\alpha\bar{\mathrm{B}}} = \alpha$, the fourth Maxwell's equation becomes

$$\nabla\times\mathbf{B} = 4\pi\alpha\mathbf{J} + \alpha\frac{\partial\mathbf{E}}{\partial t}. \tag{B.12}$$

Since $\frac{\bar{\mathrm{M}}_\mathrm{G}}{\bar{\mathrm{l}}_\mathrm{G}\cdot\bar{\mathrm{J}}_\mathrm{G}} = \frac{\bar{\mathrm{M}}}{\alpha\bar{\mathrm{l}}\cdot\bar{\mathrm{J}}} = \frac{1}{\alpha}$ and $\frac{\bar{\mathrm{P}}_\mathrm{G}}{\bar{\mathrm{t}}_\mathrm{G}\cdot\bar{\mathrm{J}}_\mathrm{G}} = \frac{\bar{\mathrm{P}}}{\bar{\mathrm{t}}\cdot\bar{\mathrm{J}}} = 1$ we can write:

$$\mathbf{J}_m = \frac{1}{\alpha}\nabla\times\mathbf{M} \tag{B.13}$$

and

$$\mathbf{J}_d = \frac{\partial\mathbf{P}}{\partial t}. \tag{B.14}$$

So the fourth macroscopic Maxwell's equation becomes

$$\nabla \times (\mathbf{B} - 4\pi\mathbf{M}) = 4\pi\alpha\mathbf{J}_f + \alpha\frac{\partial(\mathbf{E} + 4\pi\mathbf{P})}{\partial t}. \tag{B.15}$$

This suggests the definition of the magnetic field strength as $\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}$ in addition to the usual equation for the electric induction $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$. This gives:

$$\nabla \times \mathbf{H} = 4\pi\alpha\mathbf{J}_f + \alpha\frac{\partial\mathbf{D}}{\partial t}. \tag{B.16}$$

The unit of magnetic field strength is therefore derived from $\frac{\mu_0\bar{\mathrm{B}}_\mathrm{G}}{\bar{\mathrm{H}}_\mathrm{G}} = 1$ or $\frac{\bar{\mathrm{M}}_\mathrm{G}}{\bar{\mathrm{H}}_\mathrm{G}} = 4\pi$ that gives

$$\bar{\mathrm{H}}_\mathrm{G} = \mu_0\bar{\mathrm{B}}_\mathrm{G} = \alpha\mu_0\bar{\mathrm{B}} = \frac{\bar{\mathrm{M}}_\mathrm{G}}{4\pi} = \frac{1}{\alpha}\bar{\mathrm{H}} = 1.36495698941 \times 10^9 \ \mathrm{A/m}. \tag{B.17}$$

Appendix C

Magnetization Intensity

Several authors use the magnetization intensity instead of the magnetization. This quantity is defined as:

$$\mathbf{I} = \mu_0 \mathbf{M}, \tag{C.1}$$

and has the same unit of the magnetic field (Tesla T). The relationship between magnetic field strength, magnetic flux density, and magnetization intensity is written as:

$$\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{I}. \tag{C.2}$$

Appendix D

Conversion factors tables

This Appendix collects the conversion factors discussed in the text and gives their absolute and relative errors. The data reported here have been obtained with the tool `tools/units.f90` using as input the values of the first seven quantities of this list taken from the NIST web-site (`https://www.nist.gov/`). Errors are calculated from the errors of the Rydberg constant and of the fine structure constant available in the same site.
These values are updated to October 2019.

```
Experimental quantities exact in the SI:
Planck constant:            6.62607015E-34      J.s
Planck constant / 2 pi:     1.0545718176462E-34 J.s
Speed of light:             2.99792458E+08      m/s
Electron charge:            1.602176634E-19     C
Avogadro number:            6.02214076E+23
Boltzmann constant:         1.380649E-23        J/K

Approximate quantities determined by experiment:
Rydberg constant:           1.097373156816OE+07 1/m
Fine structure constant:    7.2973525693E-03
Atomic mass unit:           1.66053906660E-27   kg

Derived Physical quantities:
Electron mass:              9.1093837015E-31    kg
mu0:                        1.25663706212E-06   N/A^2
epsilon0:                   8.8541878128E-12    C^2/N m^2
E_hatree:                   4.3597447222072E-18 J
Bohr radius:                5.29177210903E-11   m
Bohr magneton:              9.2740100783E-24    J/T

Conversion factors (Atomic units - SI):
Length: \l=                 5.29177210903E-11   m
Mass: \m=                   9.1093837015E-31    kg
```

```
Mass density: \rhom=        6.1473168257E+00    kg/m^3
Time: \t=                   2.4188843265857E-17 s
Frequency: \nu=             4.1341373335182E+16 Hz
Speed: \v=                  2.18769126364E+06   m/s
Acceleration: \a=           9.0442161272E+22    m/s^2
Momentum: \p=               1.99285191410E-24   kg m/s
Angular momentum: \L=       1.0545718176462E-34 kg m^2/s
Force: \f=                  8.2387234982E-08    N
Energy: \U=                 4.3597447222072E-18 J
Power: \W=                  1.8023783420686E-01 W
Pressure: \pr=              2.9421015696E+13    Pa
Current: \I=                6.623618237510E-03  A
Charge: \C=                 1.602176634E-19     C
Charge density: \rho=       1.08120238456E+12   C/m^3
Current density: \J=        2.36533701094E+18   A/m^2
Electric field: \E=         5.14220674763E+11   N/C
Electric potential: \V=     2.7211386245988E+01 V
Capacitance: \F=            5.887890530517E-21  F
Dipole moment: \dip=        8.4783536255E-30    C m
Polarization: \P=           5.7214766229E+01    C/m^2
Electric displacement: \D= 4.5530064316E+00    C/m^2
Resistance: \R=             4.1082359022277E+03 Ohm
Magnetic induction: \B=     2.35051756758E+05   T
Vector potential: \A=       1.24384033059E-05   T m
Magnetic field flux: \Phi= 6.5821195695091E-16 Wb
Inductance: \Y=             9.937347433815E-14  H
Magnetic dipole: \mu=       1.85480201567E-23   A m^2 (J/T)
Magnetization: \M=          1.25168244230E+08   A/m
Magnetic strength: \H=      9.9605723936E+06    A/m

Conversion factors (c.g.s.-Gaussian - SI):
Length: cm=                 1.0E-02             m
Mass: g=                    1.0E-03             kg
Mass density: g/cm^3=       1.0E+03             kg/m^3
Time: s=                    1.0E+00             s
Frequency: Hz=              1.0E+00             Hz
Speed: cm/s=                1.0E-02             m/s
Acceleration: cm/s^2=       1.0E-02             m/s^2
Momentum: g cm/s=           1.0E-05             kg m/s
Angular momentum: g cm^2/s=1.0E-07             kg m^2/s
Force: dyne=                1.0E-05             N
Energy: erg=                1.0E-07             J
Power: erg/s=               1.0E-07             W
Pressure: Ba=               1.0E-01             Pa
Current: statA=             3.33564095107E-10   A
```

```
Charge: statC=              3.33564095107E-10   C
Charge density: statC/cm^3=3.33564095107E-04   C/m^3
Current density: statA/cm^2=3.33564095107E-06  A/m^2
Electric field: dyne/statC=2.99792458082E+04   N/C
Electric potential: statV= 2.99792458082E+02   V
Capacitance: cm=            1.11265005544E-12   F
Dipole moment: statC cm=    3.33564095107E-12   C m
Electric polarization: statC/cm^2= 3.33564095107E-06 C/m^2
Electric displ: statC/cm^2 4 pi = 2.65441872871E-07 C/m^2
Resistance: s/cm=           8.987551792288E+11  Ohm
Magnetic induction: G=      1.000000000274E-04  T
Vector potential: G cm=     1.000000000274E-06  T m
Magnetic field flux: Mx=    1.000000000274E-08  Wb
Inductance: statH=          8.98755179229E+11   H
Magnetic dipole: statC cm= 9.99999999726E-04   A m^2
Magnetization: statC/cm^2= 9.99999999726E+02   A/m
Magnetic strength: statC/cm^2 4 pi= 7.95774715242E+01 A/m

C/statC= 2.99792458082E+09 (C/statC)/10c= 1.00000000027E+00

mu_0/4 pi 10^-7=      1.00000000055E+00

Conversion factors (SI - c.g.s.-Gaussian):
Length: m=                  1.0E+02             cm
Mass: kg=                   1.0E+03             g
Time: s=                    1.0E+00             s
Frequency: Hz=              1.0E+00             Hz
Speed: m/s=                 1.0E+02             cm/s
Acceleration: m/s^2=        1.0E+02             cm/s^2
Momentum: kg m/s=           1.0E+05             g cm/s
Angular momentum: kg m^2/s=1.0E+07             g cm^2/s
Force: N=                   1.0E+05             dyne
Energy: J=                  1.0E+07             erg
Power: W=                   1.0E+07             erg/s
Pressure: Pa=               1.0E+01             Ba
Current: A=                 2.99792458082E+09   statA
Charge: C=                  2.99792458082E+09   statC
Charge density: C/m^3=      2.99792458082E+03   statC/cm^3
Current density: A/m^2=     2.99792458082E+05   statA/cm^2
Electric field: N/C=        3.33564095107E-05   dyne/statC
Electric potential: V=      3.33564095107E-03   statV
Capacitance: F=             8.98755179229E+11   cm
Dipole moment: C m=         2.99792458082E+11   statC cm
Electric polarization: C/m^2= 2.99792458082E+05 statC/cm^2
Electric displ.: C/m^2= 3.76730313565E+06 statC/cm^2 4pi
```

```
Resistance: Ohm=            1.112650055445E-12  s/cm
Magnetic induction: T=      9.999999997263E+03  G
Vector potential: T m=      9.999999997263E+05  G cm
Magnetic field flux: Wb=    9.999999997263E+07  Mx
Inductance: H=              1.11265005544E-12   statH
Magnetic dipole: A m^2=     1.00000000027E+03   statC cm
Magnetization: A/m=         1.00000000027E-03   statC/cm^2
Magnetic strength: A/m=     1.25663706178E-02   statC/cm^2 4pi

Conversion factors (Atomic units - c.g.s.-Gaussian):
Length:                     5.29177210903E-09   cm
Mass:                       9.1093837015E-28    g
Mass density:               6.1473168257E-03    g/cm^3
Time:                       2.4188843265857E-17 s
Frequency:                  4.1341373335182E+16 Hz
Speed:                      2.18769126364E+08   cm/s
Acceleration:               9.0442161272E+24    cm/s^2
Momentum:                   1.99285191410E-19   g cm/s
Angular momentum:           1.0545718176462E-27 g cm^2/s
Force:                      8.2387234982E-03    dyne
Energy:                     4.3597447222072E-11 erg
Power:                      1.8023783420686E+06 erg/s
Pressure:                   2.9421015696E+14    Ba
Current:                    1.98571079282E+07   statA
Charge:                     4.80320471388E-10   statC
Charge density:             3.2413632055E+15    statC/cm^3
Current density:            7.0911019670E+23    statA/cm^2
Electric field:             1.71525554062E+07   dyne/statC
Electric potential:         9.07674142975E-02   statV
Capacitance:                5.29177210903E-09   cm
Dipole moment:              2.54174647389E-18   statC cm
Polarization:               1.71525554062E+07   statC/cm^2
Electric displacement:      1.71525554062E+07   statC/cm^2 4pi
Resistance:                 4.57102890439E-09   s/cm
Magnetic induction:         2.35051756693E+09   G
Vector potential:           1.24384033025E+01   G cm
Magnetic field flux:        6.58211956771E-08   Mx
Inductance:                 1.10567901732E-25   statH
Magnetic dipole:            1.85480201618E-20   statC cm
Magnetization:              1.25168244264E+05   statC/cm^2
Magnetic strength:          1.25168244264E+05   statC/cm^2 4pi

Conversion factors (Rydberg atomic units - SI):
Length: \l_R=               5.29177210903E-11   m
Mass: \m_R=                 1.82187674030E-30   kg
```

```
Time: \t_R=                 4.8377686531714E-17 s
Frequency: \nu_R=           2.0670686667591E+16 Hz
Speed: \v_R=                1.09384563182E+06   m/s
Acceleration: \a_R=         4.52210806362E+22   m/s^2
Momentum: \p_R=             1.99285191410E-24   kg m/s
Angular momentum: \L_R=     1.0545718176462E-34 kg m^2/s
Force: \f_R=                4.11936174912E-08   N
Energy: \U_R=               2.1798723611036E-18 J
Power: \W_R=                4.50594585517lE-02  W
Pressure: \pr_R=            1.47105078482E+13   Pa
Current: \I_R=              2.3418026858671E-03 A
Charge: \C_R=               1.1329099625600E-19 C
Charge density: \rho_R=     7.6452553796E+11    C/m^3
Current density: \J_R=      8.36272920114E+17   A/m^2
Electric field: \E_R=       3.63608926151E+11   N/C
Electric potential: \V_R=   1.9241355740025E+01 V
Capacitance: \F_R=          5.887890530517E-21  F
Dipole moment: \dip_R=      5.99510134192E-30   C m
Polarization: \P_R=         4.0456949184E+01    C/m^2
Electric displacement: \D_R=3.21946172254E+00    C/m^2
Resistance: \R_R=           8.2164718044553E+03 Ohm
Magnetic induction: \B_R=   3.3241338227E+05    T
Vector potential: \A_R=     1.75905586495E-05   T m
Magnetic field flux: \Phi_R=9.3085227643611E-16 Wb
Inductance: \Y_R=           3.9749389735260E-13 H
Magnetic dipole: \mu_R=     6.5577154152E-24    A m^2 (J/T)
Magnetization: \M_R=        4.42536571420E+07   A/m
Magnetic field: \H_R=       3.52159414202E+06   A/m

Conversion factors (Gaussian atomic units - SI):
Magnetic induction: \B_G=   1.71525554109E+03   T
Vector potential: \A_G=     9.0767414322E-08    T m
Magnetic field flux: \Phi_G=4.80320471520E-18   Wb
Magnetic dipole: \mu_G=     2.5417464732E-21    A m^2 (J/T)
Magnetization: \M_G=        1.71525554016E+10   A/m
Magnetic field: \H_G=       1.36495698941E+09   A/m

Physical constants in Hartree atomic units:
Speed of light:             1.37035999084E+02
atomic mass unit:           1.8228884862E+03

Physical constants in eV:
Hartree in eV:              2.7211386246E+01
Rydberg in eV:              1.3605693123E+01
```

```
Frequency conversion:
Hz in cm^-1:                3.33564095198152E-11
cm^-1 in Hz:                2.99792458E+10

-------------------------------------------------------------
Errors:                    Absolute                  Relative

rydberg =                   2.10E-05 1/m              1.91E-12
alpha =                     1.10E-12                  1.51E-10
amu =                       5.00E-37                  3.01E-10

me =                        2.76E-40 kg               3.03E-10
abohr =                     8.08E-21 m                1.53E-10
mu0 =                       1.89E-16 N/A^2            1.51E-10
epsilon0 =                  1.33E-21 C^2/Nm^2         1.51E-10
hartree =                   8.34E-30 J                1.91E-12
bohr mag =                  2.81E-33 J/T              3.03E-10

Errors of conversion factors (atomic units - SI):
\l =                        8.08E-21 m                1.53E-10
\m =                        2.76E-40 kg               3.03E-10
\rhom =                     4.68E-09 kg/m^3           7.61E-10
\t =                        4.63E-29 s                1.91E-12
\nu =                       7.91E+04 s                1.91E-12
\v =                        3.30E-04 m/s              1.51E-10
\a =                        1.38E+13 m/s^2            1.53E-10
\p =                        3.04E-34 kg m/s           1.53E-10
\L =                        0.00E+00 kg m^2/s         0.00E+00
\f =                        1.27E-17 N                1.55E-10
\U =                        8.34E-30 J                1.91E-12
\W =                        6.90E-13 W                3.83E-12
\pr =                       1.35E+04 Pa               4.60E-10
\I =                        1.27E-14 A                1.91E-12
\C =                        0.00E+00 C                0.00E+00
\rho =                      4.95E+02 C/m^3            4.58E-10
\J =                        7.27E+08 A/m^2            3.07E-10
\E =                        7.95E+01 V/m              1.55E-10
\V =                        5.21E-11 V                1.91E-12
\F =                        1.13E-32 F                1.91E-12
\dip =                      1.29E-39 C m              1.53E-10
\P =                        1.75E-08 C/m^2            3.05E-10
\D =                        1.39E-09 C/m^2            3.05E-10
\R =                        0.00E+00 Ohm              0.00E+00
\B =                        7.18E-05 T                3.05E-10
\A =                        1.90E-15 T m              1.53E-10
```

```
\phi =                      0.00E+00 Wb              0.00E+00
\Y =                        1.90E-25 H               1.91E-12
\mu =                       5.63E-33 J/T             3.03E-10
\M =                        1.93E-02 A/m             1.55E-10
\H =                        1.54E-03 A/m             1.55E-10

cspeed =                    2.07E-08 \v              1.51E-10
amu =                       1.10E-06 \m              6.04E-10


Errors of conversion factors (c.g.s.-Gaussian - SI):
Current =                   2.51E-20 A               7.54E-11
Charge =                    2.51E-20 C               7.54E-11
Charge density =            2.51E-14 C/m^3           7.54E-11
Current density =           2.51E-16 A/m^2           7.54E-11
Electric field =            2.26E-06 V/m             7.54E-11
Electric potential =        2.26E-08 V               7.54E-11
Capacitance =               1.68E-22 F               1.51E-10
Dipole moment =             2.51E-22 C m             7.54E-11
Electric Polarization =     2.51E-16 C/m^2           7.54E-11
Electric Displacement =     2.00E-17 C/m^2           7.54E-11
Resistance =                1.35E+02 Ohm             1.51E-10
Magnetic induction =        7.54E-15 T               7.54E-11
Vector potential =          7.54E-17 T m             7.54E-11
Magnetic field flux =       7.54E-19 Wb              7.54E-11
Inductance =                1.35E+02 H               1.51E-10
Magnetic dipole =           7.54E-14 J/T             7.54E-11
Magnetization =             7.54E-08 A/m             7.54E-11
Magnetic strength =         6.00E-09 A/m             7.54E-11


Errors of conversion factors (atomic units-c.g.s.-Gaussian):
Current =                   1.53E-03 statA           7.73E-11
Charge =                    3.62E-20 statC           7.54E-11
Charge density =            1.73E+06 statC/cm^3      5.33E-10
Current density =           2.71E+14 statA/cm^2      3.83E-10
Electric field =            3.94E-03 statV/cm        2.30E-10
Electric potential =        7.01E-12 statV           7.73E-11
Capacitance =               8.08E-19 cm              1.53E-10
Dipole moment =             5.80E-28 statC cm        2.28E-10
Electric Polarization =     6.53E-03 statC/cm^2      3.81E-10
Electric displacement =     6.53E-03 statC/cm^2 4pi  3.81E-10
Resistance =                6.89E-19 s/cm            1.51E-10
Magnetic induction =        8.95E-01 G               3.81E-10
Vector potential =          2.84E-09 G cm            2.28E-10
```

```
Magnetic field flux =        4.96E-18 Mx                 7.54E-11
Inductance =                 1.69E-35 statH              1.53E-10
Magnetic dipole =            7.03E-30 statC cm           3.79E-10
Magnetization =              2.88E-05 statC/cm^2         2.30E-10
Magnetic strength =          2.88E-05 statC/cm^2 4pi     2.30E-10

Errors of conversion factors (Rydberg atomic units - SI):
\l_R =                       8.08E-21 m                  1.53E-10
\m_R =                       5.53E-40 kg                 3.03E-10
\t_R =                       9.26E-29 s                  3.83E-12
\nu_R =                      3.96E+04 s                  1.91E-12
\v_R =                       1.65E-04 m/s                1.51E-10
\a_R =                       6.90E+12 m/s^2              1.53E-10
\p_R =                       3.04E-34 kg m/s             1.53E-10
\L_R =                       0.00E+00 kg m^2/s           0.00E+00
\f_R =                       6.37E-18 N                  1.55E-10
\U_R =                       4.17E-30 J                  1.91E-12
\W_R =                       1.72E-13 W                  3.83E-12
\pr_R =                      6.76E+03 Pa                 4.60E-10
\I_R =                       4.48E-15 A                  1.91E-12
\C_R =                       0.00E+00 C                  0.00E+00
\rho_R =                     3.50E+02 C/m^3              4.58E-10
\J_R =                       2.57E+08 A/m^2              3.07E-10
\E_R =                       5.62E+01 V/m                1.55E-10
\V_R =                       5.21E-11 V                  2.71E-12
\F_R =                       1.13E-32 F                  1.91E-12
\dip_R =                     9.15E-40 C m                1.53E-10
\P_R =                       1.24E-08 C/m^2              3.05E-10
\D_R =                       9.83E-10 C/m^2              3.05E-10
\R_R =                       0.00E+00 Ohm                0.00E+00
\B_R =                       1.01E-04 T                  3.05E-10
\A_R =                       2.69E-15 T m                1.53E-10
\phi_R =                     0.00E+00 Wb                 0.00E+00
\Y_R =                       7.61E-25 H                  1.91E-12
\mu_R =                      1.99E-33 J/T                3.03E-10
\M_R =                       6.84E-03 A/m                1.55E-10
\H_R =                       5.44E-04 A/m                1.55E-10


Errors of conversion factors (Gaussian atomic units - SI):
\B_G =                       7.82E-07 T                  4.56E-10
\A_G =                       2.75E-17 T m                3.03E-10
\phi_G =                     7.24E-28 Wb                 1.51E-10
\mu_G =                      1.15E-30 J/T                4.54E-10
\M_G =                       5.24E+00 A/m                3.05E-10
```

```
\H_G =                                   4.17E-01 A/m                        3.05E-10
```

Appendix E

Bibliography

1. J.D. Jackson, Classical electrodynamics, Third edition, J. Wiley and Sons (1999).