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Overview

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Length and energy

Electric an magnetic fields

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Natural units

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October/November 2011

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• Normal matter

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Normal matter

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Normal matter

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More examples • normal matter is governed by electrostatic forces and non-relativistic quantum mechanics

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- Planck's constant

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- typical values for normal matter are reasonable numbers
- times products of powers of these constants

Constants of nature

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Constants of nature

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More examples • today, the *Système international d'unités* (SI) is in common use, in particular in science and engineering

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- today, the *Système international d'unités* (SI) is in common use, in particular in science and engineering
- also called MKSA

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- today, the *Système international d'unités* (SI) is in common use, in particular in science and engineering
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Constants of nature

- also called MKSA
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- $4\pi\epsilon_0 = 1.112650 \times 10^{-10} \text{ kg}^{-1} \text{ m}^{-3} \text{ A}^2$

Powers of MKSA

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Powers of MKSA

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- $4\pi\epsilon_0 = 1.112650 \times 10^{-10} \text{ kg}^{-1} \text{ m}^{-3} \text{ A}^2$
- the powers of SI units

	m	kg	S	Α
ħ	2	1	-1	0
e	0	0	1	1
m	0	1	0	0
$4\pi\epsilon_0$	-3	-1	4	2

Powers of natural constants

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Powers of natural constants

• the former 4×4 matrix can be inverted

Powers of natural constants

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- the former 4×4 matrix can be inverted
- SI units can be expressed as a product of powers of the involved constants of nature

	ħ	e	m	$4\pi\epsilon_0$
m	2	-2	-1	1
kg	0	0	1	0
s	3	-4	-1	2
A	-3	5	1	-2

Powers of natural constants

- the former 4×4 matrix can be inverted
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• read: s = number multiplied by $\hbar^3 e^{-4} m^{-1} (4\pi\epsilon_0)^2$ etc.

Powers of natural constants

- the former 4×4 matrix can be inverted
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m	2	-2	-1	1
kg	0	0	1	0
s	3	-4	-1	2
A	-3	5	1	-2

- read: s = number multiplied by $\hbar^3 e^{-4} m^{-1} (4\pi\epsilon_0)^2$ etc.
- find out number and exponents for arbitrary SI unit

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```
function [value,power]=atomic_unit(si)
val=[1.05457e-34,1.60218e-19,9.10938e-31,4*pi*8.85419
dim=[2 1 -1 0; 0 0 1 1; 0 1 0 0; -3 -1 4 2];
mid=round(inv(dim));
power=si*mid;
value=prod(val.^power);
```

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```
>> length = [0 1 0 0];
>> length = [1 0 0 0];
>> [astar,apow]=atomic_unit(length);
>> astar
    5.2917e-11
>> apow
    2 -2 -1 1
```

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e. g. atomic length unit

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e. g. atomic length unit

• recall length=[1 0 0 0]

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e.g. atomic length unit

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- recall length=[1 0 0 0]
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e. g. atomic length unit

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- recall length=[1 0 0 0]
- recall [astar,apow]=atomic_unit(length)
- recall astar = 5.2971e-11

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• recall length=[1 0 0 0]

- recall [astar,apow]=atomic_unit(length)
- recall astar = 5.2971e-11
- recall apow = [2 -2 -1 1]

e. g. atomic length unit

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- recall length=[1 0 0 0]
- recall [astar,apow]=atomic_unit(length)
- recall astar = 5.2971e-11
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- we have just calculated the atomic unit of length

e. g. atomic length unit

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- recall length=[1 0 0 0]
- recall [astar,apow]=atomic_unit(length)
- recall astar = 5.2971e-11
- recall apow = [2 -2 -1 1]
- · we have just calculated the atomic unit of length
- i. e. Bohr's radius

$$a_* = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 5.2917 \times 10^{-11} \text{ m}$$

e. g. atomic length unit

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Bohr's radius

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More examples • Schrödinger equation for hydrogen atom

$$-\frac{\hbar^2}{2m}\Delta\phi + \frac{1}{4\pi\epsilon_0}\frac{-e^2}{r}\phi = E\phi$$

Bohr's radius

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$$-\frac{\hbar^2}{2m}\Delta\phi+\frac{1}{4\pi\epsilon_0}\frac{-e^2}{r}\phi=E\phi$$

• in atomic units

$$-\frac{1}{2}\Delta\phi - \frac{1}{r}\phi = E\phi$$

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ground state

$$\phi \propto e^{-r}$$
 with $E = -\frac{1}{2}$

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Schrödinger equation for hydrogen atom

$$-\frac{\hbar^2}{2m}\Delta\phi+\frac{1}{4\pi\epsilon_0}\frac{-e^2}{r}\phi=E\phi$$

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• radius

$$\langle R \rangle = \frac{\int_0^\infty \mathrm{d}r \, r^2 \, e^{-r} \, r \, e^{-r}}{\int_0^\infty \mathrm{d}r \, r^2 \, e^{-r} \, 1 \, e^{-r}} = 1$$

Bohr's radius

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Schrödinger equation for hydrogen atom

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radius

$$\langle R \rangle = \frac{\int_0^\infty dr \, r^2 \, e^{-r} \, r \, e^{-r}}{\int_0^\infty dr \, r^2 \, e^{-r} \, 1 \, e^{-r}} = 1$$

• Bohr's result

$$\langle R \rangle = a_* = \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

Bohr's radius

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Hartree



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• MKSA for energy is $[2 \ 1 \ -2 \ 0]$

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- MKSA for energy is [2 1 -2 0]
- [Estar, Epow] = atomic_unit(energy)

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- MKSA for energy is [2 1 -2 0]
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- $E_* = 4.3598 \times 10^{-18} \text{ J} = 27.21 \text{ eV}$

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- atomic energy unit Hartree
- H atom ground state energy is E = -13.6 eV

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- He-Ne laser: $\lambda = 633 \text{ nm}$

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- atomic energy unit Hartree
- H atom ground state energy is E = -13.6 eV
- photon energies are in the eV range
- He-Ne laser: $\lambda = 633 \text{ nm}$
- $\hbar\omega = 0.072 E_* = 1.96 \text{ eV}$

Electric field strength

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magnetic fields

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Electric field strength

• voltage=[2 1 -3 -1]

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Electric field strength

- voltage=[2 1 -3 -1]
- el_field_str=[1 1 -3 -1]

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Electric field strength

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- voltage=[2 1 -3 -1]
- el_field_str=[1 1 -3 -1]
- the atomic (natural) unit of electric field strength is $\mathcal{E}_* = \frac{m^2 e^5}{(4\pi\epsilon_0)^3 \hbar^4} = 5.1423 \times 10^{11} \text{ V m}^{-1}$

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Electric field strength

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- Ohms law, Pockels effect, Starck effect
- external field strength is always very small

Magnetic induction

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• induction=[0 1 -2 -1]

Magnetic induction

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Magnetic induction

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- induction=[0 1 -2 -1]
- the atomic (natural) unit of magnetic induction is $\mathcal{B}_* = \frac{m^2 e^3}{(4\pi\epsilon_0)^2\hbar^3} = 2.3505 \times 10^5 \text{ T}$

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Magnetic induction

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- induction=[0 1 -2 -1]
- the atomic (natural) unit of magnetic induction is $\mathcal{R} = \frac{m^2 e^3}{m^2 e^3} = 2.2505 \times 10^5 \text{ T}$

$$\mathcal{B}_* = \frac{1}{(4\pi\epsilon_0)^2\hbar^3} = 2.3505 \times 10^5 \text{ T}$$

• Faraday effect, Hall effect ...

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- induction=[0 1 -2 -1]
- the atomic (natural) unit of magnetic induction is $\mathcal{B}_* = \frac{m^2 e^3}{(4\pi\epsilon_0)^2\hbar^3} = 2.3505 \times 10^5 \text{ T}$
- Faraday effect, Hall effect ...
- external field induction is always very small

Mass density

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• rho=[-3 1 0 0]

Mass density



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- rho=[-3 1 0 0]
- [rhoval,rhopow]=atomic_unit(rho)


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- rho=[-3 1 0 0]
- [rhoval,rhopow]=atomic_unit(rho)
- rhoval = 6.174

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- rhopow=[-6 6 4 -3]

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$$\varrho_* = \frac{m^4 e^6}{(4\pi\epsilon_0)^3\hbar^6} = \frac{m}{a_*^3} = 6.147 \text{ kg m}^{-3}$$

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Natural units

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- rho=[-3 1 0 0]
- [rhoval,rhopow]=atomic_unit(rho)
- rhoval = 6.174
- rhopow=[-6 6 4 -3]

$$\varrho_* = \frac{m^4 e^6}{(4\pi\epsilon_0)^3\hbar^6} = \frac{m}{a_*^3} = 6.147 \text{ kg m}^{-3}$$

 mass is mass of nucleons, therefore must be multiplied by approximately 4000

Light velocity

Deter Hentel			Ŭ	
Peter Herter				

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• velocity=[1 0 -1 0]

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- velocity=[1 0 -1 0]
- atomic unit of velocity is

$$v_* = \frac{e^2}{4\pi\epsilon_0\hbar} = 2.1877 \times 10^6 \text{ m s}^{-1}$$

Light velocity

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Light velocity

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Light velocity

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- velocity of light is $c = \alpha^{-1} v_*$
- fine structure constant
 - $\alpha = 1/137.035999074$

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Light velocity

relativistic corrections

Pockels coefficients

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• external electric field ${m {\cal E}}$

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- external electric field ${m {\cal E}}$
- permittivity change

$$(\epsilon(\omega; \boldsymbol{\mathcal{E}})^{-1})_{ij} = (\epsilon(\omega; 0)^{-1})_{ij} + r_{ijk}(\omega) \boldsymbol{\mathcal{E}}_k$$

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- external electric field ${\boldsymbol{\mathcal E}}$
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$$(\epsilon(\omega; \boldsymbol{\mathcal{E}})^{-1})_{ij} = (\epsilon(\omega; 0)^{-1})_{ij} + r_{ijk}(\omega)\mathcal{E}_k$$

 Pockels coefficients vanish if crystal has an inversion center

Pockels coefficients

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- Pockels coefficients vanish if crystal has an inversion center
- lithium niobate has <u>no</u> inversion center

Pockels coefficients

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- largest coefficient $r_{333} = 30 \text{ pm V}^{-1}$

Pockels coefficients

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- largest coefficient $r_{333} = 30 \text{ pm V}^{-1}$
- small or large?
- $r_{333} \, \mathcal{E}_* \approx 16$
- · lithium niobate is rather resilient to electrical fields

Pockels coefficients

Elasticity module

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Elasticity module

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More examples • An elastic medium is described by stress and strain



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- An elastic medium is described by stress and strain
- strain tensor S_{ij} describes deformation

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- An elastic medium is described by stress and strain
- strain tensor S_{ij} describes deformation
- stress tensor T_{ij} describes force on area element

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- $\mathrm{d}F_j = \mathrm{d}A_iT_{ij}$

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- $\mathrm{d}F_j = \mathrm{d}A_iT_{ij}$
- Hooke's law

$$T_{ij} = \frac{E}{1+\nu} \left\{ S_{ij} + \frac{\nu}{1-2\nu} \delta_{ij} S_{kk} \right\}$$

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Elasticity module

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• Poisson's ratio between 0 and 1/2

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- Poisson's ratio between 0 and 1/2
- elasticity module E

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- expect $E = \text{eV} \text{ Å}^{-3} = 160 \text{ GPa}$

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Elasticity module

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- Poisson's ratio between 0 and 1/2
- elasticity module E
- expect $E = \text{eV} \text{ Å}^{-3} = 160 \text{ GPa}$
- ... as order of magnitude
- steel : E = 200 GPa

Elasticity module

Susceptibility

Feter Herter

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• Recall the Drude model result $\chi(\omega) = \chi(0) \frac{\Omega^2}{\Omega^2 - \omega^2 - i\Gamma\omega}$



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- Recall the Drude model result $\chi(\omega) = \chi(0) \frac{\Omega^2}{\Omega^2 \omega^2 i\Gamma\omega}$
- where

$$\chi(0) = \frac{Nq^2}{\epsilon_0 m \Omega^2}$$

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recall

$$m(\ddot{\boldsymbol{x}} + \Gamma \dot{\boldsymbol{x}} + \Omega^2 \boldsymbol{x}) = q\boldsymbol{E}$$

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recall

$$m(\ddot{\boldsymbol{x}} + \Gamma \dot{\boldsymbol{x}} + \Omega^2 \boldsymbol{x}) = q\boldsymbol{E}$$

• $N \approx 1$ and $\Omega \approx 1$ in natural units!

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