Equations in Physics

By ir. J.C.A. Wevers

Contents

Physical Constants

Name	Symbol	Value	Unit
Number π	π	3,14159265	
Number e	e	2,718281828459	
Euler's constant	$\gamma = \lim\limits_{n\to\infty}\left(\sum\limits_{k=1}^{n} 1/k - \ln(n)\right) = 0,5772156649$		
Elementary charge	e	$1,60217733 \cdot 10^{-19}$	C
Gravitational constant	G, κ	$6,67259 \cdot 10^{-11}$	$\mathrm{m^3kg^{-1}s^{-2}}$
Fine-structure constant	$\alpha = e^2/2hc\varepsilon_0$	$\approx 1/137$	
Speed of light in vacuum	c	$2,99792458 \cdot 10^{8}$	m/s (def)
Permittivity of the vacuum	ε_0	$8,854187 \cdot 10^{-12}$	F/m
Permeability of the vacuum	μ_0	$4\pi \cdot 10^{-7}$	H/m
$(4\pi\varepsilon_0)^{-1}$		$8,9876 \cdot 10^{9}$	$\mathrm{Nm^2C^{-2}}$
Planck's constant	h	$6,6260755 \cdot 10^{-34}$	Js
Dirac's constant	$\hbar = h/2\pi$	$1,0545727 \cdot 10^{-34}$	Js
Bohr magneton	$\mu_\mathrm{B} = e\hbar/2m_\mathrm{e}$	$9,2741 \cdot 10^{-24}$	$\mathrm{Am^2}$
Bohr radius	a_0	$0,52918$	Å
Rydberg's constant	Ry	13,595	eV
Electron Compton wavelength	$\lambda_\mathrm{Ce} = h/m_\mathrm{e}c$	$2,2463 \cdot 10^{-12}$	m
Proton Compton wavelength	$\lambda_\mathrm{Cp} = h/m_\mathrm{p}c$	$1,3214 \cdot 10^{-15}$	m
Reduced mass of the H-atom	μ_H	$9,1045755 \cdot 10^{-31}$	kg
Stefan-Boltzmann's constant	σ	$5,67032 \cdot 10^{-8}$	$\mathrm{Wm^2K^{-4}}$
Wien's constant	k_W	$2,8978 \cdot 10^{-3}$	mK
Molar gasconstant	R	8,31441	J/mol
Avogadro's constant	N_A	$6,0221367 \cdot 10^{23}$	$\mathrm{mol^{-1}}$
Boltzmann's constant	$k = R/N_\mathrm{A}$	$1,380658 \cdot 10^{-23}$	J/K
Electron mass	m_e	$9,1093897 \cdot 10^{-31}$	kg
Proton mass	m_p	$1,6726231 \cdot 10^{-27}$	kg
Neutron mass	m_n	$1,674954 \cdot 10^{-27}$	kg
Elementary mass unit	$m_\mathrm{u} = \frac{1}{12}m(^{12}_{6}\mathrm{C})$	$1,6605656 \cdot 10^{-27}$	kg
Nuclear magneton	μ_N	$5,0508 \cdot 10^{-27}$	J/T
Diameter of the Sun	$D_\odot$	$1392 \cdot 10^{6}$	m
Mass of the Sun	$M_\odot$	$1,989 \cdot 10^{30}$	kg
Rotational period of the Sun	$T_\odot$	25,38	days
Radius of Earth	R_A	$6,378 \cdot 10^{6}$	m
Mass of Earth	M_A	$5,976 \cdot 10^{24}$	kg
Rotational period of Earth	T_A	23,96	hours
Astronomical unit	AU	$1,4959787066 \cdot 10^{11}$	m
Light year	lj	$9,4605 \cdot 10^{15}$	m
Parsec	pc	$3,0857 \cdot 10^{16}$	m
Hubble constant	H	$\approx (75 \pm 25)$	$\mathrm{km{\cdot}s^{-1}{\cdot}Mpc^{-1}}$

Chapter 1

Mechanics

1.1 Point-kinetics in a fixed coordinate system

1.1.1 Definitions

The position $\vec{r}$, the velocity $\vec{v}$ and the acceleration $\vec{a}$ are defined by: $\vec{r} = (x, y, z)$, $\vec{v} = (\dot{x}, \dot{y}, \dot{z})$, $\vec{a} = (\ddot{x}, \ddot{y}, \ddot{z})$. The following holds:

$$s(t) = s_0 + \int |\vec{v}(t)| dt \ ; \quad \vec{r}(t) = \vec{r}_0 + \int \vec{v}(t) dt \ ; \quad \vec{v}(t) = \vec{v}_0 + \int \vec{a}(t) dt$$

When the acceleration is constant this gives: $v(t) = v_0 + at$ and $s(t) = s_0 + v_0 t + \frac{1}{2}at^2$.
For the unit vectors in a direction $\perp$ to the orbit $\vec{e}_\mathrm{t}$ and parallel to it $\vec{e}_\mathrm{n}$ holds:

$$\vec{e}_\mathrm{t} = \frac{\vec{v}}{|\vec{v}|} = \frac{d\vec{r}}{ds} \quad \dot{\vec{e}}_\mathrm{t} = \frac{v}{\rho}\vec{e}_\mathrm{n} \ ; \quad \vec{e}_\mathrm{n} = \frac{\dot{\vec{e}}_\mathrm{t}}{|\dot{\vec{e}}_\mathrm{t}|}$$

For the *curvature* k and the *radius of curvature* ρ holds:

$$\vec{k} = \frac{d\vec{e}_\mathrm{t}}{ds} = \frac{d^2\vec{r}}{ds^2} = \left| \frac{d\varphi}{ds} \right| \ ; \quad \rho = \frac{1}{|k|}$$

1.1.2 Polar coordinates

Polar coordinates are defined by: $x = r\cos(\theta)$, $y = r\sin(\theta)$. So, for the unit coordinate vectors holds: $\dot{\vec{e}}_r = \dot{\theta}\vec{e}_\theta$, $\dot{\vec{e}}_\theta = -\dot{\theta}\vec{e}_r$

The velocity and the acceleration are derived from: $\vec{r} = r\vec{e}_r$, $\vec{v} = \dot{r}\vec{e}_r + r\dot{\theta}\vec{e}_\theta$, $\vec{a} = (\ddot{r} - r\dot{\theta}^2)\vec{e}_r + (2\dot{r}\dot{\theta} + r\ddot{\theta})\vec{e}_\theta$.

1.2 Relative motion

For the motion of a point D w.r.t. a point Q holds: $\vec{r}_\mathrm{D} = \vec{r}_\mathrm{Q} + \dfrac{\vec{\omega} \times \vec{v}_\mathrm{Q}}{\omega^2}$ with $\vec{\mathrm{QD}} = \vec{r}_\mathrm{D} - \vec{r}_\mathrm{Q}$ and $\omega = \dot{\theta}$.

Further holds: $\alpha = \ddot{\theta}$. $'$ means that the quantity is defined in a moving system of coordinates. In a moving system holds:
$\vec{v} = \vec{v}_\mathrm{Q} + \vec{v}\,' + \vec{\omega} \times \vec{r}\,'$ and $\vec{a} = \vec{a}_\mathrm{Q} + \vec{a}\,' + \vec{\alpha} \times \vec{r}\,' + 2\vec{\omega} \times \vec{v} - \vec{\omega} \times (\vec{\omega} \times \vec{r}\,')$
with $|\vec{\omega} \times (\vec{\omega} \times \vec{r}\,')| = \omega^2 \vec{r}_n\,'$

1.3 Point-dynamics in a fixed coordinate system

1.3.1 Force, (angular)momentum and energy

Newton's 2nd law connects the force on an object and the resulting acceleration of the object:

$$\vec{F}(\vec{r}, \vec{v}, t) = m\vec{a} = \frac{d\vec{p}}{dt} \ \text{, where the } \textit{momentum} \text{ is given by: } \ \vec{p} = m\vec{v}$$

Newton's 3rd law is: $\vec{F}_\mathrm{action} = -\vec{F}_\mathrm{reaction}$.

For the power P holds: $P=\dot{W}=\vec{F}\cdot\vec{v}$. For the total energy W, the kinetic energy T and the potential energy U holds: $W=T+U$; $\quad\dot{T}=-\dot{U}$ with $T=\frac{1}{2}mv^2$.

The *kick* $\vec{S}$ is given by: $\vec{S}=\Delta\vec{p}=\int\vec{F}dt$

The work A, delivered by a force, is $A=\int\limits_1^2\vec{F}\cdot d\vec{s}=\int\limits_1^2 F\cos(\alpha)ds$

The torque $\vec{\tau}$ is related to the angular momentum $\vec{L}$: $\vec{\tau}=\dot{\vec{L}}=\vec{r}\times\vec{F}$; and $\vec{L}=\vec{r}\times\vec{p}=m\vec{v}\times\vec{r}$, $|\vec{L}|=mr^2\omega$. The following holds:

$$\tau=-\frac{\partial U}{\partial\theta}$$

So, the conditions for a mechanical equilibrium are: $\sum\vec{F}_i=0$ and $\sum\vec{\tau}_i=0$.

The *force of friction* is usually proportional with the force perpendicular to the surface, except when the motion starts, when a threshold has to be overcome: $F_{\rm fric}=f\cdot F_{\rm norm}\cdot\vec{e}_{\rm t}$.

1.3.2 Conservative force fields

A conservative force can be written as the gradient of a potential: $\vec{F}_{\rm cons}=-\vec{\nabla}U$. From this follows that rot$\vec{F}=\vec{0}$. For such a force field also holds:

$$\oint\vec{F}\cdot d\vec{s}=0\ \Rightarrow\ U=U_0-\int\limits_{r_0}^{r_1}\vec{F}\cdot d\vec{s}$$

So the work delivered by a conservative force field depends not on the followed trajectory but only on the starting and ending points of the motion.

1.3.3 Gravitation

The Newtonian law of gravitation is (in GRT one also uses κ instead of G):

$$\vec{F}_{\rm g}=-G\frac{m_1m_2}{r^2}\vec{e}_r$$

The gravitationpotential is then given by $V=-Gm/r$. From Gauss law then follows: $\nabla^2V=4\pi G\varrho$.

1.3.4 Orbital equations

From the equations of Lagrange for ϕ, conservation of angular momentum can be derived:

$$\frac{\partial\mathcal{L}}{\partial\phi}=\frac{\partial V}{\partial\phi}=0\Rightarrow\frac{d}{dt}(mr^2\phi)=0\Rightarrow L_z=mr^2\phi=\text{constant}$$

For the radius as a function of time can be found that:

$$\left(\frac{dr}{dt}\right)^2=\frac{2(W-V)}{m}-\frac{L^2}{m^2r^2}$$

The angular equation is then:

$$\phi-\phi_0=\int\limits_0^r\left[\frac{mr^2}{L}\sqrt{\frac{2(W-V)}{m}-\frac{L^2}{m^2r^2}}\right]^{-1}dr\overset{r^{-2}\text{field}}{=}\arccos\left(1+\frac{\frac{1}{r}-\frac{1}{r_0}}{\frac{1}{r_0}+km/L_z^2}\right)$$

if $F=F(r)$: $L=$constant, if F is conservative: $W=$constant, if $\vec{F}\perp\vec{v}$ then $\Delta T=0$ and $U=0$.

Kepler's equations

In a force field $F = kr^{-2}$, the orbits are conic sections (Kepler's 1st law). The equation of the orbit is:

$$r(\theta) = \frac{\ell}{1 + \varepsilon\cos(\theta - \theta_0)} \ , \ \text{ or: } \ x^2 + y^2 = (\ell - \varepsilon x)^2$$

with

$$\ell = \frac{L^2}{G\mu^2 M_{\rm tot}} \ ; \quad \varepsilon^2 = 1 + \frac{2WL^2}{G^2\mu^3 M_{\rm tot}^2} = 1 - \frac{\ell}{a} \ ; \quad a = \frac{\ell}{1-\varepsilon^2} = \frac{k}{2W}$$

a is half the length of the long axis of the elliptical orbit in case the orbit is closed. Half the length of the short axis is $b = \sqrt{a\ell}$. ε is the *excentricity* of the orbit. Orbits with an equal ε are equally shaped. Now, 5 kinds of orbits are possible:

1. $k < 0$ and $\varepsilon = 0$: a circle.
2. $k < 0$ and $0 < \varepsilon < 1$: an ellipse.
3. $k < 0$ and $\varepsilon = 1$: a parabole.
4. $k < 0$ and $\varepsilon > 1$: a hyperbole, curved towards the center of force.
5. $k > 0$ and $\varepsilon > 1$: a hyperbole, curved away of the center of force.

Other combinations are not possible: the total energy in a repulsive force field is always positive so $\varepsilon > 1$.

If the surface between the orbit walked thru between t_1 and t_2 and the focus C around which the planet moves is $A(t_1, t_2)$, Kepler's 2nd law is

$$A(t_1, t_2) = \frac{L_{\rm C}}{2m}(t_2 - t_1)$$

Kepler's 3rd law is, with T the period and $M_{\rm tot}$ the total mass of the system:

$$\frac{T^2}{a^3} = \frac{4\pi^2}{GM_{\rm tot}}$$

1.3.5 The virial theorem

The virial theorem for one particle is:

$$\langle m\vec{v}\cdot\vec{r}\rangle = 0 \Rightarrow \langle T\rangle = -\tfrac{1}{2}\left\langle \vec{F}\cdot\vec{r}\right\rangle = \tfrac{1}{2}\left\langle r\frac{dU}{dr}\right\rangle = \tfrac{1}{2}n\langle U\rangle \ \text{ if } U = -\frac{k}{r^n}$$

The virial theorem for a collection of particles is:

$$\langle T\rangle = -\tfrac{1}{2}\left\langle \sum_{\rm particles}\vec{F}_i\cdot\vec{r}_i + \sum_{\rm pairs}\vec{F}_{ij}\cdot\vec{r}_{ij}\right\rangle$$

These propositions can also be written as: $2E_{\rm kin} + E_{\rm pot} = 0$.

1.4 Point dynamics in a moving coordinate system

1.4.1 Apparent forces

The total force in a moving coordinate system can be found by subtracting the apparent forces from the forces working in the reference frame: $\vec{F}\,' = \vec{F} - \vec{F}_{\rm app}$. The different apparent forces are given by:

1. Transformation of the origin: $F_{\rm or} = -m\vec{a}_a$

2. Rotation: $\vec{F}_\alpha = -m\vec{\alpha} \times \vec{r}\,'$
3. Coriolis force: $F_{\rm cor} = -2m\vec{\omega} \times \vec{v}$
4. Centrifugal force: $\vec{F}_{\rm cf} = m\omega^2\vec{r}_n\,' = -\vec{F}_{\rm cp}$; $\vec{F}_{\rm cp} = -\dfrac{mv^2}{r}\vec{e}_r$

1.4.2 Tensor notation

Transformation of the Newtonian equations of motion to $x^\alpha = x^\alpha(x)$ gives:

$$\frac{dx^\alpha}{dt} = \frac{\partial x^\alpha}{\partial \bar{x}^\beta}\frac{d\bar{x}^\beta}{dt};$$

so

$$\frac{d}{dt}\frac{dx^\alpha}{dt} = \frac{d^2x^\alpha}{dt^2} = \frac{d}{dt}\left(\frac{\partial x^\alpha}{\partial \bar{x}^\beta}\frac{d\bar{x}^\beta}{dt}\right) = \frac{\partial x^\alpha}{\partial \bar{x}^\beta}\frac{d^2\bar{x}^\beta}{dt^2} + \frac{d\bar{x}^\beta}{dt}\frac{d}{dt}\left(\frac{\partial x^\alpha}{\partial \bar{x}^\beta}\right)$$

The chain rule gives:

$$\frac{d}{dt}\frac{\partial x^\alpha}{\partial \bar{x}^\beta} = \frac{\partial}{\partial \bar{x}^\gamma}\frac{\partial x^\alpha}{\partial \bar{x}^\beta}\frac{d\bar{x}^\gamma}{dt} = \frac{\partial^2 x^\alpha}{\partial \bar{x}^\beta \partial \bar{x}^\gamma}\frac{d\bar{x}^\gamma}{dt}$$

So:

$$\frac{d^2x^\alpha}{dt^2} = \frac{\partial x^\alpha}{\partial \bar{x}^\beta}\frac{d^2\bar{x}^\beta}{dt^2} + \frac{\partial^2 x^\alpha}{\partial \bar{x}^\beta \partial \bar{x}^\gamma}\frac{d\bar{x}^\gamma}{dt}$$

So the Newtonian equation of motion

$$m\frac{d^2x^\alpha}{dt^2} = F^\alpha$$

will be transformed into:

$$m\left\{\frac{d^2x^\alpha}{dt^2} + \Gamma^\alpha_{\beta\gamma}\frac{dx^\beta}{dt}\frac{dx^\gamma}{dt}\right\} = F^\alpha$$

The apparent forces are brought from he origin to the effect side in the way $\Gamma^\alpha_{\beta\gamma}\dfrac{dx^\beta}{dt}\dfrac{dx^\gamma}{dt}$.

1.5 Dynamics of masspoint collections

1.5.1 The center of mass

The velocity w.r.t. the center of mass $\vec{R}$ is given by $\vec{v} - \dot{\vec{R}}$. The coordinates of the center of mass are given by:

$$\vec{r}_{\rm m} = \frac{\sum m_i\vec{r}_i}{\sum m_i}$$

In a 2-particle system, the coordinates of the center of mass are given by:

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$$

With $\vec{r} = \vec{r}_1 - \vec{r}_2$, the kinetic energy becomes: $T = \frac{1}{2}M_{\rm tot}\dot{R}^2 + \frac{1}{2}\mu\dot{r}^2$, with the *reduced mass* μ is given by: $\dfrac{1}{\mu} = \dfrac{1}{m_1} + \dfrac{1}{m_2}$

The motion within and outside the center of mass can be separated:

$$\dot{\vec{L}}_{\rm outside} = \vec{\tau}_{\rm outside} \ ; \quad \dot{\vec{L}}_{\rm inside} = \vec{\tau}_{\rm inside}$$

$$\vec{p} = m\vec{v}_{\rm m} \ ; \quad \vec{F}_{\rm ext} = m\vec{a}_{\rm m} \ ; \quad \vec{F}_{12} = \mu\vec{u}$$

1.5.2 Collisions

With collisions, where B are the coordinates of the collision and C an arbitrary other position, holds: $\vec{p} = m\vec{v}_{\rm m}$ is constant, and $T = \frac{1}{2}m\vec{v}_{\rm m}^{\,2}$ is constant. The changes in the *relative velocities* can be derived from: $\vec{S} = \Delta\vec{p} = \mu(\vec{v}_{\rm aft} - \vec{v}_{\rm before})$. Further holds $\Delta\vec{L}_{\rm C} = \vec{\rm CB} \times \vec{S}$, $\vec{p} \parallel \vec{S}$ =constant and $\vec{L}$ w.r.t. B is constant.

1.6 Dynamics of rigid bodies

1.6.1 Moment of Inertia

The angular momentum in a moving coordinate system is given by:

$$\vec{L}' = I\vec{\omega} + \vec{L}'_n$$

where I is the *moment of inertia* with respect to a central axis, which is given by:

$$I = \sum_i m_i \vec{r}_i^{\;2} \;\; ; \quad T' = W_{\rm rot} = \tfrac{1}{2}\omega I_{ij}\vec{e}_i\vec{e}_j = \tfrac{1}{2}I\omega^2$$

or, in the continuous case:

$$I = \frac{m}{V}\int r'_n dV = \int r'_n dm$$

Further holds:

$$L_i = I^{ij}\omega_j \;\; ; \quad I_{ii} = I_i \;\; ; \quad I_{ij} = I_{ji} = -\sum_k m_k x'_i x'_j$$

Steiner's theorem is: $I_{\rm w.r.t.D} = I_{\rm w.r.t.C} + m(DM)^2$ if axis C $\parallel$ axis D.

Object	I	Object	I
Cavern cylinder	$I = mR^2$	Massive cylinder	$I = \frac{1}{2}mR^2$
Disc, axis in plane disc through m	$I = \frac{1}{4}mR^2$	Halter	$I = \frac{1}{2}\mu R^2$
Cavern sphere	$I = \frac{2}{3}mR^2$	Massive sphere	$I = \frac{2}{5}mR^2$
Bar, axis $\perp$ through c.o.m.	$I = \frac{1}{12}ml^2$	Bar, axis $\perp$ through end	$I = \frac{1}{3}ml^2$
Rectangle, axis $\perp$ plane thr. c.o.m.	$I = \frac{1}{12}(a^2 + b^2)$	Rectangle, axis $\parallel$ b thr. m	$I = ma^2$

1.6.2 Principal axes

Each rigid body has (at least) 3 principal axes which stand $\perp$ at each other. For a principal axis holds:

$$\frac{\partial I}{\partial \omega_x} = \frac{\partial I}{\partial \omega_y} = \frac{\partial I}{\partial \omega_z} = 0 \;\text{ so }\; L'_n = 0$$

The following holds: $\dot{\omega}_k = -a_{ijk}\omega_i\omega_j$ with $a_{ijk} = \dfrac{I_i - I_j}{I_k}$ if $I_1 \leq I_2 \leq I_3$.

1.6.3 Time dependence

For torque of force $\vec{\tau}$ holds:

$$\vec{\tau}\,' = I\ddot{\theta} \;\; ; \quad \frac{d''\vec{L}'}{dt} = \vec{\tau}\,' - \vec{\omega} \times \vec{L}'$$

The *torque* $\vec{T}$ is defined by: $\vec{T} = \vec{F} \times \vec{d}$.

1.7 Variational Calculus, Hamilton and Lagrange mechanics

1.7.1 Variational Calculus

Starting with:

$$\delta\int\limits_a^b \mathcal{L}(q,\dot{q},t)dt=0 \ \text{ met } \ \delta(a)=\delta(b)=0 \ \text{ and } \ \delta\left(\frac{du}{dx}\right)=\frac{d}{dx}(\delta u)$$

the equations of Lagrange can be derived:

$$\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{q}_i}=\frac{\partial\mathcal{L}}{\partial q_i}$$

When there are additional conditions applying on the variational problem $\delta J(u)=0$ of the type $K(u)$ =constant, the new problem becomes: $\delta J(u)-\lambda\delta K(u)=0$.

1.7.2 Hamilton mechanics

The *Lagrangian* is given by: $\mathcal{L}=\sum T(\dot{q}_i)-V(q_i)$. The *Hamiltonian* is given by: $H=\sum\dot{q}_ip_i-\mathcal{L}$. In 2 dimensions holds: $\mathcal{L}=T-U=\frac{1}{2}m(\dot{r}^2+r^2\dot{\phi}^2)-U(r,\phi)$.

If the used coordinates are *canonical* are the Hamilton equations the equations of motion for the system:

$$\frac{dq_i}{dt}=\frac{\partial H}{\partial p_i}\ ;\quad \frac{dp_i}{dt}=-\frac{\partial H}{\partial q_i}$$

Coordinates are canonical if the following holds: $\{q_i,q_j\}=0$, $\{p_i,p_j\}=0$, $\{q_i,p_j\}=\delta_{ij}$ where $\{,\}$ is the *Poisson bracket*:

$$\{A,B\}=\sum_i\left[\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}-\frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right]$$

1.7.3 Motion around an equilibrium, linearization

For natural systems around equilibrium holds:

$$\left(\frac{\partial V}{\partial q_i}\right)_0=0\ ;\quad V(q)=V(0)+V_{ik}q_iq_k \ \text{ with } \ V_{ik}=\left(\frac{\partial^2V}{\partial q_i\partial q_k}\right)_0$$

With $T=\frac{1}{2}(M_{ik}\dot{q}_i\dot{q}_k)$ one receives the set of equations $M\ddot{q}+Vq=0$. If we substitute $q_i(t)=a_i\exp(i\omega t)$, this set of equations has solutions if $\det(V-\omega^2M)=0$. This leads to the eigenfrequentions of the problem: $\omega_k^2=\dfrac{a_k^{\rm T}Va_k}{a_k^{\rm T}Ma_k}$. If the equilibrium is stable holds: $\forall k$ that $\omega_k^2>0$. The general solution is a superposition if eigenvibrations.

1.7.4 Phase space, Liouville's equation

In phase space holds:

$$\nabla=\left(\sum_i\frac{\partial}{\partial q_i},\sum_i\frac{\partial}{\partial p_i}\right) \ \text{ so } \ \nabla\cdot\vec{v}=\sum_i\left(\frac{\partial}{\partial q_i}\frac{\partial H}{\partial p_i}-\frac{\partial}{\partial p_i}\frac{\partial H}{\partial q_i}\right)$$

If the equation of continuity, $\partial_t\varrho+\nabla\cdot(\varrho\vec{v})=0$ holds, this can be written as:

$$\{\varrho,H\}+\frac{\partial\varrho}{\partial t}=0$$

For an arbitrary quantity A holds:

$$\frac{dA}{dt}=\{A,H\}+\frac{\partial A}{\partial t}$$

Liouville's theorem can than be written as:

$$\frac{d\varrho}{dt}=0~;\quad\text{or:}~\int pdq=\text{constant}$$

1.7.5 Generating functions

Starting with the coordinate transformation:

$$\left\{\begin{array}{l}Q_i=Q_i(q_i,p_i,t)\\P_i=P_i(q_i,q_i,t)\end{array}\right.$$

The following Hamilton equations can be derived:

$$\frac{dQ_i}{dt}=\frac{\partial K}{\partial P_i}~;\quad\frac{dP_i}{dt}=-\frac{\partial K}{\partial Q_i}$$

Now, a distinction between 4 cases can be made:

1. If $p_i\dot{q}_i-H=P_iQ_i-K(P_i,Q_i,t)-\dfrac{dF_1(q_i,Q_i,t)}{dt}$, the coordinates follow from:

$$p_i=\frac{\partial F_1}{\partial q_i}~;\quad P_i=\frac{\partial F_1}{\partial Q_i}~;\quad K=H+\frac{dF_1}{dt}$$

2. If $p_i\dot{q}_i-H=-\dot{P}_iQ_i-K+\dfrac{dF_2(q_i,P_i,t)}{dt}$, the coordinates follow from:

$$p_i=\frac{\partial F_2}{\partial q_i}~;\quad Q_i=\frac{\partial F_2}{\partial P_i}~;\quad K=H+\frac{\partial F_2}{\partial t}$$

3. If $-\dot{p}_iq_i-H=P_i\dot{Q}_i-K+\dfrac{dF_3(p_i,Q_i,t)}{dt}$, the coordinates follow from:

$$q_i=-\frac{\partial F_3}{\partial p_i}~;\quad P_i=-\frac{\partial F_3}{\partial Q_i}~;\quad K=H+\frac{\partial F_3}{\partial t}$$

4. If $-\dot{p}_iq_i-H=-P_iQ_i-K+\dfrac{dF_4(p_i,P_i,t)}{dt}$, the coordinates follow from:

$$q_i=-\frac{\partial F_4}{\partial p_i}~;\quad Q_i=\frac{\partial F_4}{\partial p_i}~;\quad K=H+\frac{\partial F_4}{\partial t}$$

The functions F_1, F_2, F_3 and F_4 are called *generating functions*.

The Hamiltonian of a charged particle with charge q in an external electromagnetic field is given by:

$$H=\frac{1}{2m}\left(\vec{p}-q\vec{A}\right)^2+qV$$

This Hamiltonian can be derived from the Hamiltonian of a free particle $H=p^2/2m$ with the transformations $\vec{p}\rightarrow\vec{p}-q\vec{A}$ and $H\rightarrow H-qV$. This is elegant from a relativistic point of view: this is equivalent with the transformation of the momentum 4-vector $p^\alpha\rightarrow p^\alpha-qA^\alpha$. A gaugetransformation on the potentials A^α corresponds with a canonical transformation, which make the Hamilton equations the equations of motion for the system.

Chapter 2

Electricity & Magnetism

2.1 The Maxwell equations

The classical electromagnetic field can be described with the *Maxwell equations*, and can be written both as differential and integral equations:

$$\begin{array}{ll}
\displaystyle\oiint (\vec{D}\cdot\vec{n})d^2A = Q_{\rm free,included} & \nabla\cdot\vec{D} = \rho_{\rm free} \\
\displaystyle\oiint (\vec{B}\cdot\vec{n})d^2A = 0 & \nabla\cdot\vec{B} = 0 \\
\displaystyle\oint \vec{E}\cdot d\vec{s} = -\frac{d\Phi}{dt} & \displaystyle\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t} \\
\displaystyle\oint \vec{H}\cdot d\vec{s} = I_{\rm free,included} + \frac{d\Psi}{dt} & \displaystyle\nabla\times\vec{H} = \vec{J}_{\rm free} + \frac{\partial\vec{D}}{\partial t}
\end{array}$$

For the fluxes holds: $\Psi = \iint (\vec{D}\cdot\vec{n})d^2A$, $\Phi = \iint (\vec{B}\cdot\vec{n})d^2A$.

The electric displacement $\vec{D}$, polarization $\vec{P}$ and electric field strength $\vec{E}$ depend on each other according to:

$\vec{D} = \varepsilon_0\vec{E} + \vec{P} = \varepsilon_0\varepsilon_{\rm r}\vec{E}$, $\vec{P} = \sum\vec{p}_0/{\rm Vol}$, $\varepsilon_{\rm r} = 1 + \chi_{\rm e}$, with $\chi_{\rm e} = \dfrac{np_0^2}{3\varepsilon_0 kT}$

The magnetic field strength $\vec{H}$, the magnetization $\vec{M}$ and the magnetic flux density $\vec{B}$ depend on each other according to:

$\vec{B} = \mu_0(\vec{H} + \vec{M}) = \mu_0\mu_{\rm r}\vec{H}$, $\vec{M} = \sum\vec{m}/{\rm Vol}$, $\mu_{\rm r} = 1 + \chi_{\rm m}$, with $\chi_{\rm m} = \dfrac{\mu_0 n m_0^2}{3kT}$

2.2 Force and potential

The force and the electric field between 2 point charges are given by:

$$\vec{F}_{12} = \frac{Q_1Q_2}{4\pi\varepsilon_0\varepsilon_{\rm r}r^2}\vec{e}_r\ ; \quad \vec{E} = \frac{\vec{F}}{Q}$$

The Lorentzforce is the force which is felt by a charged particle that moves through a magnetic field. The origin of this force is a relativistic transformation of the Coulomb force: $\vec{F}_{\rm L} = Q(\vec{v}\times\vec{B}) = l(\vec{I}\times\vec{B})$.

The magnetic field which results from an electric current is given by the law of Biot-Savart:

$$d\vec{B} = \frac{\mu_0 I}{4\pi r^2}d\vec{l}\times\vec{e}_r$$

If the current is time-dependent one has to take *retardation* into account: the substitution $I(t) \to I(t - r/c)$ has to be applied.

The potentials are given by:

$$V_{12} = -\int\limits_1^2 \vec{E}\cdot d\vec{s}\ , \quad \vec{A} = \tfrac{1}{2}\vec{B}\times\vec{r}$$

Here, the freedom remains to apply a *gauge transformation.* The fields can be derived from the potentials as follows:

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t} \ , \quad \vec{B} = \nabla \times \vec{A}$$

Further holds the relation: $c^2\vec{B} = \vec{v} \times \vec{E}$.

2.3 Gauge transformations

The potentials of the electromagnetic fields transform as follows when a gauge transformation is applied:

$$\left\{ \begin{array}{l} \vec{A}' = \vec{A} - \nabla f \\ V' = V + \dfrac{\partial f}{\partial t} \end{array} \right.$$

so the fields $\vec{E}$ and $\vec{B}$ do not change. This results in a canonical transformation of the Hamiltonian. Further, the freedom remains to apply a limiting condition. Two common choices are:

1. Lorentz-gauge: $\nabla \cdot \vec{A} + \dfrac{1}{c^2}\dfrac{\partial V}{\partial t} = 0$. This separates the differential equations for $\vec{A}$ and V: $\Box V = -\dfrac{\rho}{\varepsilon_0}$, $\Box \vec{A} = -\mu_0 \vec{J}$.
2. Coulomb gauge: $\nabla \cdot \vec{A} = 0$. If $\rho = 0$ and $\vec{J} = 0$ holds $V = 0$ and follows $\vec{A}$ from $\Box \vec{A} = 0$.

2.4 Energy of the electromagnetic field

The energy density of the electromagnetic field is:

$$\frac{dW}{d\text{Vol}} = w = \int HdB + \int EdD$$

The energy density can be expressed in the potentials and currents as follows:

$$w_{\text{mag}} = \tfrac{1}{2}\int \vec{J} \cdot \vec{A} d^3x \ \ , \ \ w_{\text{el}} = \tfrac{1}{2}\int \rho V d^3x$$

2.5 Electromagnetic waves

2.5.1 Electromagnetic waves in vacuum

The wave equation $\Box\Psi(\vec{r},t) = -f(\vec{r},t)$ has the general solution, with $c = (\varepsilon_0\mu_0)^{-1/2}$:

$$\Psi(\vec{r},t) = \int \frac{f(\vec{r}, t - |\vec{r} - \vec{r}\,'|/c)}{4\pi|\vec{r} - \vec{r}\,'|} d^3r'$$

If this is written as: $\vec{J}(\vec{r},t) = \vec{J}(\vec{r})\exp(-i\omega t)$ and $\vec{A}(\vec{r},t) = \vec{A}(\vec{r})\exp(-i\omega t)$ with:

$$\vec{A}(\vec{r}) = \frac{\mu}{4\pi}\int \vec{J}(\vec{r}\,')\frac{\exp(ik|\vec{r} - \vec{r}\,'|)}{|\vec{r} - \vec{r}\,'|}d^3\vec{r}\,' \ \ , \quad V(\vec{r}) = \frac{1}{4\pi\varepsilon}\int \rho(\vec{r}\,')\frac{\exp(ik|\vec{r} - \vec{r}\,'|)}{|\vec{r} - \vec{r}\,'|}d^3\vec{r}\,'$$

will a derivation via multipole development show that for the radiated energy holds, if $d, \lambda \gg r$:

$$\frac{dP}{d\Omega} = \frac{k^2}{32\pi^2\varepsilon_0 c}\left|\int J_\perp(\vec{r}\,')e^{i\vec{k}\cdot\vec{r}}d^3r'\right|^2$$

The energy density of the electromagnetic wave of a vibrating dipole at a large distance is:

$$w = \varepsilon_0 E^2 = \frac{p_0^2\sin^2(\theta)\omega^4}{16\pi^2\varepsilon_0 r^2 c^4}\sin^2(kr - \omega t) \ , \quad \langle w \rangle_t = \frac{p_0^2\sin^2(\theta)\omega^4}{32\pi^2\varepsilon_0 r^2 c^4} \ , \quad P = \frac{ck^4|\vec{p}\,|^2}{12\pi\varepsilon_0}$$

The radiated energy can be derived from the *Poynting vector* $\vec{S}$: $\vec{S}=\vec{E}\times\vec{H}=cW\vec{e}_v$. The *irradiance* is the time-averaged of the Poynting vector: $I=\langle|\vec{S}|\rangle_t$. The radiation pressure p_s is given by $p_\mathrm{s}=(1+R)|\vec{S}|/c$, where R is the coefficient of reflection.

2.5.2 Electromagnetic waves in mater

The wave equations in matter, with $c_\mathrm{mat}=(\varepsilon\mu)^{-1/2}$ are:

$$\left(\nabla^2-\varepsilon\mu\frac{\partial^2}{\partial t^2}-\frac{\mu}{\rho}\frac{\partial}{\partial t}\right)\vec{E}=0\ ,\ \ \left(\nabla^2-\varepsilon\mu\frac{\partial^2}{\partial t^2}-\frac{\mu}{\rho}\frac{\partial}{\partial t}\right)\vec{B}=0$$

give, after substitution of monochromatic plane waves: $\vec{E}=E\exp(i(\vec{k}\cdot\vec{r}-\omega t))$ and $\vec{B}=B\exp(i(\vec{k}\cdot\vec{r}-\omega t))$ the dispersion relation:

$$k^2=\varepsilon\mu\omega^2+\frac{i\mu\omega}{\rho}$$

The first term arises from the displacement current, the second from the conductance current. If k is written as $k:=k'+ik''$ holds:

$$k'=\omega\sqrt{\tfrac{1}{2}\varepsilon\mu}\sqrt{1+\sqrt{1+\frac{1}{(\rho\varepsilon\omega)^2}}}\quad\text{and}\quad k''=\omega\sqrt{\tfrac{1}{2}\varepsilon\mu}\sqrt{-1+\sqrt{1+\frac{1}{(\rho\varepsilon\omega)^2}}}$$

This results in a damped wave: $\vec{E}=E\exp(-k''\vec{n}\cdot\vec{r})\exp(i(k'\vec{n}\cdot\vec{r}-\omega t))$. If the material is a good conductor, the wave vanishes after approximately one wavelength, $k=(1+i)\sqrt{\dfrac{\mu\omega}{2\rho}}$.

2.6 Multipoles

Because $\dfrac{1}{|\vec{r}-\vec{r}\,'|}=\dfrac{1}{r}\sum\limits_0^\infty\left(\dfrac{r'}{r}\right)^l P_l(\cos\theta)$ can the potential be written as: $V=\dfrac{Q}{4\pi\varepsilon}\sum\limits_n\dfrac{k_n}{r^n}$

For the lowest-order terms this results in:

- Monopole: $l=0$, $k_0=\int\rho dV$
- Dipole: $l=1$, $k_1=\int r\cos(\theta)\rho dV$
- Quadrupole: $l=2$, $k_2=\frac{1}{2}\sum\limits_i(3z_i^2-r_i^2)$

1. The electric dipole: dipolemoment: $\vec{p}=Ql\vec{e}$, where $\vec{e}$ goes from $\oplus$ to $\ominus$, and $\vec{F}=(\vec{p}\cdot\nabla)\vec{E}_\mathrm{ext}$, and $W=-\vec{p}\cdot\vec{E}_\mathrm{out}$.
   Electric field: $\vec{E}\approx\dfrac{Q}{4\pi\varepsilon r^3}\left(\dfrac{3\vec{p}\cdot\vec{r}}{r^2}-\vec{p}\right)$. The torque is: $\vec{\tau}=\vec{p}\times\vec{E}_\mathrm{out}$
2. The magnetic dipole: dipolemoment: if $r\gg\sqrt{A}$: $\vec{\mu}=\vec{I}\times(A\vec{e}_\perp)$, $\vec{F}=(\vec{\mu}\cdot\nabla)\vec{B}_\mathrm{out}$
   $|\mu|=\dfrac{mv_\perp^2}{2B}$, $W=-\vec{\mu}\times\vec{B}_\mathrm{out}$
   Magnetic field: $\vec{B}=\dfrac{-\mu}{4\pi r^3}\left(\dfrac{3\mu\cdot\vec{r}}{r^2}-\vec{\mu}\right)$. The moment is: $\vec{\tau}=\vec{\mu}\times\vec{B}_\mathrm{out}$

2.7 Electric currents

The continuity equation for charge is: $\dfrac{\partial\rho}{\partial t}+\nabla\cdot\vec{J}=0$. The *electric current* is given by:

$$I=\frac{dQ}{dt}=\iint(\vec{J}\cdot\vec{n})d^2A$$

For most conductors holds: $\vec{J}=\vec{E}/\rho$, where ρ is the *resistivity*.

If the flux enclosed by a conductor changes this results in an *induction voltage* $V_{\rm ind}=-N\dfrac{d\Phi}{dt}$. If the current flowing through a conductor changes, this results in a self-inductance voltage which works against the change: $V_{\rm selfind}=-L\dfrac{dI}{dt}$. If a conductor encloses a flux Φ holds: $\Phi=LI$.

The magnetic induction within a coil is approximated by: $B=\dfrac{\mu NI}{\sqrt{l^2+4R^2}}$ where l is the length, R the radius and N the number of coils. The energy contained within a coil is given by $W=\frac{1}{2}LI^2$ and $L=\mu N^2A/l$.

The *Capacity* is defined by: $C=Q/V$. For a capacitor holds: $C=\varepsilon_0\varepsilon_{\rm r}A/d$ where d is the distance between the plates and A the surface of one plate. The electric field strength between the plates is $E=\sigma/\varepsilon_0=Q/\varepsilon_0A$ where σ is the surface charge. The accumulated energy is given by $W=\frac{1}{2}CV^2$. The current through a capacity is given by $I=-C\dfrac{dV}{dt}$.

For most PTC resistors holds approximately: $R=R_0(1+\alpha T)$, where $R_0=\rho l/A$. For a NTC holds: $R(T)=C\exp(-B/T)$ where B and C depend only on the material.

If a current flows through two different, connecting conductors x and y, the contact area will heat up or cool down, depending on the direction of the current: the *Peltier effect*. The generated or removed heat is given by: $W=\Pi_{xy}It$. This effect can be amplified with semiconductors.

The *thermic voltage* between 2 metals is given by: $V=\gamma(T-T_0)$. For a Cu-Konstantane connection holds: $\gamma\approx 0,2-0.7$ mV/K.

In an electrical net with only stationary currents, *Kirchhoff's* equations apply: for a knot holds: $\sum I_n=0$, along a closed path holds: $\sum V_n=\sum I_nR_n=0$.

2.8 Depolarizing field

If a dielectric material is placed in an electric or magnetic field, the field strength within and outside the material will change because the material will be polarized or magnetized. If the medium has an ellipsoidal shape and one of the principal axes are parallel with the external field $\vec{E}_0$ or $\vec{B}_0$ is the depolarizing field homogeneous.

$$\begin{aligned}\vec{E}_{\rm dep}&=\vec{E}_{\rm mat}-\vec{E}_0=-\frac{\mathcal{N}\vec{P}}{\varepsilon_0}\\ \vec{H}_{\rm dep}&=\vec{H}_{\rm mat}-\vec{H}_0=-\mathcal{N}\vec{M}\end{aligned}$$

$\mathcal{N}$ is a constant depending only on the shape of the object placed in the field, with $0\leq\mathcal{N}\leq 1$. For a few limiting cases of an ellipsoid holds: a thin plane: $\mathcal{N}=1$, a long, thin bar: $\mathcal{N}=0$, a sphere: $\mathcal{N}=\frac{1}{3}$.

2.9 Mixtures of materials

The average electric displacement in a material which in inhomogenious on a mesoscopic scale is given by: $\langle D\rangle=\langle\varepsilon E\rangle=\varepsilon^*\langle E\rangle$ where $\varepsilon^*=\varepsilon_1\left(1-\dfrac{\phi_2(1-x)}{\Phi(\varepsilon^*/\varepsilon_2)}\right)^{-1}$ where $x=\varepsilon_1/\varepsilon_2$. For a sphere holds: $\Phi=\frac{1}{3}+\frac{2}{3}x$. Further holds:

$$\left(\sum_i\frac{\phi_i}{\varepsilon_i}\right)^{-1}\leq\varepsilon^*\leq\sum_i\phi_i\varepsilon_i$$

Chapter 3

Relativity

3.1 Special relativity

3.1.1 The Lorentz transformation

The Lorentz transformation $(\vec{x}\,', t') = (\vec{x}\,'(\vec{x}, t), t'(\vec{x}, t))$ leaves the wave equation invariant if c is invariant:

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} = \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t'^2}$$

This transformation can also be found when $ds^2 = ds'^2$ is demanded. The general form of the Lorentz transformation is given by:

$$\vec{x}\,' = \vec{x} + \frac{(\gamma - 1)(\vec{x} \cdot \vec{v})\vec{v}}{|v|^2} - \gamma\vec{v}t \quad , \quad t' = \frac{\gamma(t - \vec{x} \cdot \vec{v})}{c^2}$$

where

$$\gamma = \frac{1}{\sqrt{1 - \dfrac{v^2}{c^2}}}$$

If the velocity is parallel to the x-axis, this becomes:

$$\begin{aligned} x' &= \gamma(x - vt) & x &= \gamma(x' + vt') \\ y' &= y & z' &= z \\ t' &= \gamma\left(t - \frac{xv}{c^2}\right) & t &= \gamma\left(t' + \frac{x'v}{c^2}\right) \end{aligned}$$

The velocity difference $\vec{v}\,'$ between two observers transforms according to:

$$\vec{v}\,' = \left(\gamma\left(1 - \frac{\vec{v}_1 \cdot \vec{v}_2}{c^2}\right)\right)^{-1}\left(\vec{v}_2 + (\gamma - 1)\frac{\vec{v}_1 \cdot \vec{v}_2}{v_2^2}\vec{v}_1 - \gamma\vec{v}_1\right)$$

If $\vec{v} = v\vec{e}_x$ holds:

$$p_x' = \gamma\left(p_x - \frac{\beta W}{c}\right) \quad , \quad W' = \gamma(W - vp_x)$$

With $\beta = v/c$ the electric field of a moving charge is given by:

$$\vec{E} = \frac{Q}{4\pi\varepsilon_0 r^2}\frac{(1 - \beta^2)\vec{e}_r}{(1 - \beta^2\sin^2(\theta))^{3/2}}$$

The electromagnetic field transforms according to:

$$\vec{E}\,' = \gamma(\vec{E} + \vec{v} \times \vec{B})' \quad , \quad \vec{B}\,' = \gamma\left(\vec{B} - \frac{\vec{v} \times \vec{E}}{c^2}\right)$$

Length, mass and time transform according to: $\Delta t_{\rm b} = \gamma\Delta t_{\rm e}$, $m_{\rm b} = \gamma m_0$, $l_{\rm b} = l_0/\gamma$, with ${}_{\rm e}$ the quantities *in* the frame of he observer and ${}_{\rm b}$ the quantities outside it. The proper time τ is defined as: $d\tau^2 = ds^2/c^2$, so $\Delta\tau = \Delta t/\gamma$. For energy and momentum holds: $W = mc^2 = \gamma W_0$, $W^2 = m_0^2c^4 + p^2c^2$. $p = mv = Wv/c^2$, and $pc = W\beta$ where $\beta = v/c$.

4-vectors have the property that their modulus is independent of the observer: their components *can* change after a coordinate transformation but not their modulus. The difference of two 4-vectors transforms also as a 4-vector. The 4-vector for the velocity is given by $U^\alpha = \frac{dx^\alpha}{d\tau}$. The relation with the "common" velocity $u^i := dx^i/dt$ is: $U^\alpha = (\gamma u^i, ic\gamma)$. For particles with nonzero restmass holds: $U^\alpha U_\alpha = -c^2$, for particles with zero restmass (so with $v = c$) holds: $U^\alpha U_\alpha = 0$. The 4-vector for energy and momentum is given by: $p^\alpha = m_0 U^\alpha = (\gamma p^i, iW/c)$. So: $p_\alpha p^\alpha = -m_0^2 c^2 = p^2 - W^2/c^2$.

3.1.2 Red and blue shift

There are three causes of red and blue shifts:

1. Motion: with $\vec{e}_v \cdot \vec{e}_r = \cos(\varphi)$ follows: $\frac{f'}{f} = \gamma \left(1 - \frac{v\cos(\varphi)}{c}\right)$.
   This can give both red- and blueshift, also ⊥ the direction of motion.
2. Gravitational redshift: $\frac{\Delta f}{f} = \frac{\kappa M}{rc^2}$.
3. Redshift because the universe expands, resulting in e.g. the cosmic background radiation: $\frac{\lambda_0}{\lambda_1} = \frac{R_0}{R_1}$.

3.1.3 The stress-energy tensor and the field tensor

The stress-energy tensor is given by:

$$T_{\mu\nu} = (\varrho c^2 + p)u_\mu u_\nu + p g_{\mu\nu} + \frac{1}{c^2}\left(F^\mu_\alpha F^{\alpha\nu} + \tfrac{1}{4} g^{\mu\nu} F^{\alpha\beta} F_{\alpha\beta}\right)$$

The conservation laws can than be written as: $\nabla_\nu T^{\mu\nu} = 0$. The electromagnetic field tensor is given by:

$$\boxed{F_{\alpha\beta} = \frac{\partial A_\beta}{\partial x^\alpha} - \frac{\partial A_\alpha}{\partial x^\beta}}$$

with $A_\mu := (\vec{A}, iV/c)$ and $J_\mu := (\vec{J}, ic\rho)$. The Maxwell equations can than be written as:

$$\partial_\nu F^{\mu\nu} = \mu_0 J^\mu \ , \quad \partial_\lambda F_{\mu\nu} + \partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} = 0$$

The equations of motion for a charged particle in an EM field become with the field tensor:

$$\boxed{\frac{dp_\alpha}{d\tau} = qF_{\alpha\beta}u^\beta}$$

3.2 General relativity

3.2.1 Riemannian geometry, the Einstein tensor

The basic principles of general relativity are:

1. The geodesic postulate: free falling particles move along geodesics of space-time with the proper time τ or arc length s as parameter. For particles with zero rest mass (photons), the use of a free parameter is required because for them holds $ds = 0$. From $\delta \int ds = 0$ the equations of motion can be derived:
   $$\frac{d^2 x^\alpha}{ds^2} + \Gamma^\alpha_{\beta\gamma} \frac{dx^\beta}{ds}\frac{dx^\gamma}{ds} = 0$$
2. The *principle of equivalence*: inertial mass ≡ gravitational mass ⇒ gravitation is equivalent with a curved space-time were particles move along geodesics.

3. By a proper choice of the coordinate system it is possible to make the metric locally flat in each point x_i: $g_{\alpha\beta}(x_i)=\eta_{\alpha\beta}$:=diag$(-1,1,1,1)$.

The *Riemann tensor* is defined as: $R^\mu_{\nu\alpha\beta}T^\nu:=\nabla_\alpha\nabla_\beta T^\mu-\nabla_\beta\nabla_\alpha T^\mu$, where the covariant derivate is given by $\nabla_j a^i=\partial_j a^i+\Gamma^i_{jk}a^k$ and $\nabla_j a_i=\partial_j a_i-\Gamma^k_{ij}a_k$. Here,

$$\Gamma^i_{jk}=\frac{\partial^2\bar{x}^l}{\partial x^j\partial x^k}\frac{\partial x^i}{\partial\bar{x}^l}$$

are the *Christoffel symbols*. For a second-order tensor holds: $[\nabla_\alpha,\nabla_\beta]T^\mu_\nu=R^\mu_{\sigma\alpha\beta}T^\sigma_\nu+R^\sigma_{\nu\alpha\beta}T^\mu_\sigma$, $\nabla_k a^i_j=\partial_k a^i_j-\Gamma^l_{kj}a^i_l+\Gamma^i_{kl}a^l_j$, $\nabla_k a_{ij}=\partial_k a_{ij}-\Gamma^l_{ki}a_{lj}-\Gamma^l_{kj}a_{jl}$ and $\nabla_k a^{ij}=\partial_k a^{ij}+\Gamma^i_{kl}a^{lj}+\Gamma^j_{kl}a^{il}$. The following holds: $R^\alpha_{\beta\mu\nu}=\partial_\mu\Gamma^\alpha_{\beta\nu}-\partial_\nu\Gamma^\alpha_{\beta\mu}+\Gamma^\alpha_{\sigma\mu}\Gamma^\sigma_{\beta\nu}-\Gamma^\alpha_{\sigma\nu}\Gamma^\sigma_{\beta\mu}$.

The *Ricci tensor* is a contraction of the Riemann tensor: $R_{\alpha\beta}:=R^\mu_{\alpha\mu\beta}$, which is symmetric: $R_{\alpha\beta}=R_{\beta\alpha}$. The *Bianchi identities* are: $\nabla_\lambda R_{\alpha\beta\mu\nu}+\nabla_\nu R_{\alpha\beta\lambda\mu}+\nabla_\mu R_{\alpha\beta\nu\lambda}=0$.

The *Einstein tensor* is given by: $G^{\alpha\beta}:=R^{\alpha\beta}-\frac{1}{2}g^{\alpha\beta}R$, where $R:=R^\alpha_\alpha$ is the *Ricci scalar*, for which holds: $\nabla_\beta G_{\alpha\beta}=0$. With the variational principle $\delta\int(\mathcal{L}(g_{\mu\nu})-Rc^2/16\pi\kappa)\sqrt{|g|}d^4x=0$ for variations $g_{\mu\nu}\to g_{\mu\nu}+\delta g_{\mu\nu}$ the *Einstein field equations* can be derived:

$$\boxed{G_{\alpha\beta}=\frac{8\pi\kappa}{c^2}T_{\alpha\beta}}\quad\text{, which can also be written as}\quad R_{\alpha\beta}=\frac{8\pi\kappa}{c^2}(T_{\alpha\beta}-\tfrac{1}{2}g_{\alpha\beta}T^\mu_\mu)$$

For empty space this is equivalent with $R_{\alpha\beta}=0$. The equation $R_{\alpha\beta\mu\nu}=0$ has as only solution a flat space.

The Einstein equations are of 10 independent equations, who are second order in $g_{\mu\nu}$. From here, the Laplace equation from Newtonian gravitation can be derived by stating: $g_{\mu\nu}=\eta_{\mu\nu}+h_{\mu\nu}$, where $|h|\ll1$. In the stationary case, this results in $\nabla^2h_{00}=8\pi\kappa\varrho/c^2$.

The most general shape of the field equations is: $R_{\alpha\beta}-\frac{1}{2}g_{\alpha\beta}R+\Lambda g_{\alpha\beta}=\dfrac{8\pi\kappa}{c^2}T_{\alpha\beta}$

where Λ is the *cosmological constant*. This constant plays a role in inflatory models of the universe.

3.2.2 The line element

The *metric tensor* is given by: $g_{ij}=\displaystyle\sum_k\frac{\partial\bar{x}^k}{\partial x^i}\frac{\partial\bar{x}^k}{\partial x^j}$.

In general holds: $ds^2=g_{\mu\nu}dx^\mu dx^\nu$. In special relativity this becomes $ds^2=-c^2dt^2+dx^2+dy^2+dz^2$. This metric, $\eta_{\mu\nu}$:=diag$(-1,1,1,1)$, is called the *Minkowski metric*.

The *external Schwarzschild metric* applies in vacuum outside a spherical mass distribution, and is given by:

$$ds^2=\left(-1+\frac{2m}{r}\right)c^2dt^2+\left(1-\frac{2m}{r}\right)^{-1}dr^2+r^2d\Omega^2$$

Here, $m:=M\kappa/c^2$ is the *geometrical mass* of an object with mass M, and $d\Omega^2=d\theta^2+\sin^2\theta d\varphi^2$. This metric is singular for $r=2m=2\kappa M/c^2$. If an object is smaller than its eventhorizon $2m$ it is called a *black hole*. The Newtonian limit of this metric is given by:

$$ds^2=-(1+2V)c^2dt^2+(1-2V)(dx^2+dy^2+dz^2)$$

where $V=-\kappa M/r$ is the Newtonian gravitation potential. In general relativity, the components of $g_{\mu\nu}$ are associated with the potentials and the derivates of $g_{\mu\nu}$ with the field strength.

The Kruskal-Szekeres coordinates are used to solve certain problems with the Schwarzschild metric near $r=2m$. They are defined by:

- $r > 2m$:

$$\left\{\begin{array}{lcl} u &=& \sqrt{\dfrac{r}{2m}-1}\exp\left(\dfrac{r}{4m}\right)\cosh\left(\dfrac{t}{4m}\right)\\ v &=& \sqrt{\dfrac{r}{2m}-1}\exp\left(\dfrac{r}{4m}\right)\sinh\left(\dfrac{t}{4m}\right)\end{array}\right.$$

- $r < 2m$:

$$\left\{\begin{array}{lcl} u &=& \sqrt{1-\dfrac{r}{2m}}\exp\left(\dfrac{r}{4m}\right)\sinh\left(\dfrac{t}{4m}\right)\\ v &=& \sqrt{1-\dfrac{r}{2m}}\exp\left(\dfrac{r}{4m}\right)\cosh\left(\dfrac{t}{4m}\right)\end{array}\right.$$

- $r = 2m$: here, the Kruskal coordinates are singular, which is necessary to eliminate the coordinate singularity there.

The line element in these coordinates is given by:

$$ds^2 = -\frac{32m^3}{r}\mathrm{e}^{-r/2m}(dv^2 - du^2) + r^2 d\Omega^2$$

The line $r = 2m$ corresponds to $u = v = 0$, the limit $x^0 \to \infty$ with $u = v$ and $x^0 \to -\infty$ with $u = -v$. The Kruskal coordinates are only singular on the hyperbole $v^2 - u^2 = 1$, this corresponds with $r = 0$. On the line $dv = \pm du$ holds $d\theta = d\varphi = ds = 0$.

For the metric outside a rotating, charged spherical mass the Newman metric applies:

$$\begin{array}{rcl} ds^2 &=& \left(1-\dfrac{2mr-e^2}{r^2+a^2\cos^2\theta}\right)c^2dt^2 - \left(\dfrac{r^2+a^2\cos^2\theta}{r^2-2mr+a^2-e^2}\right)dr^2 - (r^2+a^2\cos^2\theta)d\theta^2 - \\ && \left(r^2+a^2+\dfrac{(2mr-e^2)a^2\sin^2\theta}{r^2+a^2\cos^2\theta}\right)\sin^2\theta d\varphi^2 + \left(\dfrac{2a(2mr-e^2)}{r^2+a^2\cos^2\theta}\right)\sin^2\theta(d\varphi)(cdt)\end{array}$$

where $m = \kappa M/c^2$, $a = L/Mc$ and $e = \kappa Q/\varepsilon_0 c^2$.

3.2.3 Planetary orbits and the perihelium shift

To find a planetary orbit, the variational problem $\delta\int ds = 0$ has to be solved. This is equivalent with the problem $\delta\int ds^2 = \delta\int g_{ij}dx^i dx^j = 0$. Substituting the external Schwarzschild metric gives for a planetary orbit:

$$\frac{du}{d\varphi}\left(\frac{d^2u}{d\varphi^2}+u\right) = \frac{du}{d\varphi}\left(3mu + \frac{m}{h^2}\right)$$

where $u := 1/r$ and $h = r^2\dot{\varphi}$ =constant. The term $3mu$ is not present in the classical solution. This term can in the classical case also be found with a potential $V(r) = -\dfrac{\kappa M}{r}\left(1+\dfrac{h^2}{r^2}\right)$.

The orbital equation gives r =constant as solution, or can, after dividing by $du/d\varphi$, be solved with perturbation theory. In zeroth order, this results in an elliptical orbit: $u_0(\varphi) = A + B\cos(\varphi)$ with $A = m/h^2$ and B an arbitrary constant. In first order, this becomes:

$$u_1(\varphi) = A + B\cos(\varphi - \varepsilon\varphi) + \varepsilon\left(A + \frac{B^2}{2A} - \frac{B^2}{6A}\cos(2\varphi)\right)$$

where $\varepsilon = 3m^2/h^2$ is small. The perihelion of a planet is the point for which r is minimal, or u maximal. This is the case if $\cos(\varphi - \varepsilon\varphi) = 0 \Rightarrow \varphi \approx 2\pi n(1+\varepsilon)$. For the perihelion shift then follows: $\Delta\varphi = 2\pi\varepsilon = 6\pi m^2/h^2$ per orbit.

3.2.4 The trajectory of a photon

For the trajectory of a photon (and for each particle with zero restmass) holds $ds^2 = 0$. Substituting the external Schwarzschild metric results in the following orbital equation:

$$\frac{du}{d\varphi}\left(\frac{d^2u}{d\varphi^2} + u - 3mu\right) = 0$$

3.2.5 Gravitational waves

Starting with the approximation $g_{\mu\nu} = \eta_{\mu\nu} + h_{\mu\nu}$ for weak gravitational fields, and the definition $h'_{\mu\nu} = h_{\mu\nu} - \frac{1}{2}\eta_{\mu\nu}h^\alpha_\alpha$, follows that $\Box h'_{\mu\nu} = 0$ if the gauge condition $\partial h'_{\mu\nu}/\partial x^\nu = 0$ is satisfied. From this, it follows that the loss of energy of a mechanical system, if the occurring velocities are $\ll c$ and for wavelengths $\gg$ the size of the system, is given by:

$$\frac{dE}{dt} = -\frac{G}{5c^5}\sum_{i,j}\left(\frac{d^3Q_{ij}}{dt^3}\right)^2$$

with $Q_{ij} = \int \varrho(x_ix_j - \frac{1}{3}\delta_{ij}r^2)d^3x$ the mass quadrupole moment.

3.2.6 Cosmology

If for the universe as a whole is assumed:

1. There exists a global time coordinate which acts as x^0 of a Gaussian coordinate system,
2. The 3-dimensional spaces are isotrope for a certain value of x^0,
3. Each point is equivalent to each other point for a fixed x^0.

then the *Robertson-Walker metric* can be derived for the line element:

$$ds^2 = -c^2dt^2 + \frac{R^2(t)}{r_0^2\left(1 - \dfrac{kr^2}{4r_0^2}\right)}(dr^2 + r^2d\Omega^2)$$

For the *scalefactor* $R(t)$ the following equations can be derived:

$$\frac{2\ddot{R}}{R} + \frac{\dot{R}^2 + kc^2}{R^2} = -\frac{8\pi\kappa p}{c^2} \quad \text{and} \quad \frac{\dot{R}^2 + kc^2}{R^2} = \frac{8\pi\kappa\varrho}{3}$$

where p is the pressure and ϱ the density of the universe. For the *deceleration parameter* q follows from this:

$$q = -\frac{\ddot{R}R}{\dot{R}^2} = \frac{4\pi\kappa\varrho}{3H^2}$$

where $H = \dot{R}/R$ is *Hubble's constant.* This is a measure of the velocity of which galaxies far away are moving away of each other, and has the value $\approx (75 \pm 25)$ km·s^{-1}·Mpc^{-1}. This gives 3 possible conditions of the universe (here, W is the total amount of energy in the universe):

1. Parabolical universe: $k = 0$, $W = 0$, $q = \frac{1}{2}$. The expansion velocity of the universe $\rightarrow 0$ if $t \rightarrow \infty$. The hereto related density $\varrho_c = 3H^2/8\pi\kappa$ is the *critical density.*
2. Hyperbolical universe: $k = -1$, $W < 0$, $q < \frac{1}{2}$. The expansion velocity of the universe remains positive forever.
3. Elliptical universe: $k = 1$, $W > 0$, $q > \frac{1}{2}$. The expansion velocity of the universe becomes negative after some time: the universe starts falling together.

Chapter 4

Oscillations

4.1 Harmonic oscillations

The general shape of a harmonic oscillation is: $\Psi(t) = \hat{\Psi}\mathrm{e}^{i(\omega t \pm \varphi)} \equiv \hat{\Psi}\cos(\omega t \pm \varphi)$,

where $\hat{\Psi}$ is the *amplitude*. A superposition of more harmonic oscillations with the same frequency results in an other harmonic oscillation:

$$\sum_i \hat{\Psi}_i \cos(\alpha_i \pm \omega t) = \hat{\Phi}\cos(\beta \pm \omega t)$$

with:

$$\tan(\beta) = \frac{\sum\limits_i \hat{\Psi}_i \sin(\alpha_i)}{\sum\limits_i \hat{\Psi}_i \cos(\alpha_i)} \quad \text{and} \quad \hat{\Phi}^2 = \sum_i \hat{\Psi}_i^2 + 2\sum_{j>i}\sum_i \hat{\Psi}_i\hat{\Psi}_j\cos(\alpha_i - \alpha_j)$$

For harmonic oscillations holds: $\displaystyle\int x(t)dt = \frac{x(t)}{i\omega}$ and $\displaystyle\frac{d^n x(t)}{dt^n} = (i\omega)^n x(t)$.

4.2 Mechanic oscillations

For a construction with a spring with constant C parallel to a damping k which is connected to a mass M, on which a periodic force $F(t) = \hat{F}\cos(\omega t)$ is applied holds the equation of motion $m\ddot{x} = F(t) - k\dot{x} - Cx$. With complex amplitudes, this becomes $-m\omega^2 x = F - Cx - ik\omega x$. With $\omega_0^2 = C/m$ follows:

$$x = \frac{F}{m(\omega_0^2 - \omega^2) + ik\omega} \quad \text{,and for the velocity holds: } \dot{x} = \frac{F}{i\sqrt{Cm}\delta + k}$$

where $\delta = \dfrac{\omega}{\omega_0} - \dfrac{\omega_0}{\omega}$. The quantity $Z = F/\dot{x}$ is called the *impedance* of the system. The *quality* of the system is given by $Q = \dfrac{\sqrt{Cm}}{k}$.

The frequency with minimal $|Z|$ is called *velocity resonance frequency*. This is equal to ω_0. In the *resonance curve* is $|Z|/\sqrt{Cm}$ plotted against ω/ω_0. The width of this curve is characterized by the points where $|Z(\omega)| = |Z(\omega_0)|\sqrt{2}$. In these points holds: $R = X$ and $\delta = \pm Q^{-1}$, and the width is $2\Delta\omega_{\mathrm{B}} = \omega_0/Q$.

The *stiffness* of an oscillating system is given by F/x. The *amplitude resonance frequency* ω_{A} is the frequency where $i\omega Z$ is minimal. This is the case for $\omega_{\mathrm{A}} = \omega_0\sqrt{1 - \frac{1}{2}Q^2}$.

The *damping frequency* ω_{D} is a measure for the time in which an oscillating system comes to rest. It is given by $\omega_{\mathrm{D}} = \omega_0\sqrt{1 - \dfrac{1}{4Q^2}}$. A weak damped oscillation ($k^2 < 4mC$) dies after $T_{\mathrm{D}} = 2\pi/\omega_{\mathrm{D}}$. For a *critical damped* oscillation ($k^2 = 4mC$) holds $\omega_{\mathrm{D}} = 0$. A strong damped oscillation ($k^2 > 4mC$) drops like (if $k^2 \gg 4mC$) $x(t) \approx x_0\exp(-t/\tau)$.

4.3 Electric oscillations

The *impedance* is given by: $Z = R + iX$. The phase angle is $\varphi := \arctan(X/R)$. The impedance of a resistor is R, of a capacitor $1/i\omega C$ and of a self inductor $i\omega L$. The quality of a coil is $Q = \omega L/R$. The total impedance in case several elements are positioned is given by:

1. Series connection: $V = IZ$,

$$Z_{\rm tot} = \sum_i Z_i \ , \quad L_{\rm tot} = \sum_i L_i \ , \quad \frac{1}{C_{\rm tot}} = \sum_i \frac{1}{C_i} \ , \quad Q = \frac{Z_0}{R} \ , \quad Z = R(1 + iQ\delta)$$

2. parallel connection: $V = IZ$,

$$\frac{1}{Z_{\rm tot}} = \sum_i \frac{1}{Z_i} \ , \quad \frac{1}{L_{\rm tot}} = \sum_i \frac{1}{L_i} \ , \quad C_{\rm tot} = \sum_i C_i \ , \quad Q = \frac{R}{Z_0} \ , \quad Z = \frac{R}{1 + iQ\delta}$$

Here, $Z_0 = \sqrt{\dfrac{L}{C}}$ and $\omega_0 = \dfrac{1}{\sqrt{LC}}$.

The power given by a source is given by $P(t) = V(t) \cdot I(t)$, so
$\langle P \rangle_t = \frac{1}{2}\hat{V}\hat{I}\cos(\phi_v - \phi_i) = \hat{V}_{\rm eff}\hat{I}_{\rm eff}\cos(\Delta\phi)$ where $\cos(\Delta\phi)$ is the work factor.

4.4 Waves in long conductors

These cables are in use for signal transfer, e.g. coax cable. For them holds: $Z_0 = \sqrt{\dfrac{dL}{dx}\dfrac{dx}{dC}}$.
The transmission velocity is given by $v = \sqrt{\dfrac{dx}{dL}\dfrac{dx}{dC}}$.

4.5 Coupled conductors and transformers

For two coils enclosing each others flux holds: if Φ_{12} is the part of the flux originating from I_2 through coil 2 which is enclosed by coil 1, than holds $\Phi_{12} = M_{12}I_2$, $\Phi_{21} = M_{21}I_1$. For the coefficients of mutual induction M_{ij} holds:

$$M_{12} = M_{21} := M = k\sqrt{L_1 L_2} = \frac{N_1\Phi_1}{I_2} = \frac{N_2\Phi_2}{I_1} \sim N_1 N_2$$

where $0 \leq k \leq 1$ is the *coupling factor*. For a transformer it is $k \approx 1$. At full load holds:

$$\frac{V_1}{V_2} = \frac{I_2}{I_1} = -\frac{i\omega M}{i\omega L_2 + R_{\rm load}} \approx -\sqrt{\frac{L_1}{L_2}} = -\frac{N_1}{N_2}$$

4.6 Pendulums

The oscillation time $T = 1/f$, and for different types of pendulums is given by:

- Oscillating spring: $T = 2\pi\sqrt{m/C}$ if the spring force is given by $F = C \cdot \Delta l$.
- Physical pendulum: $T = 2\pi\sqrt{I/\tau}$ with τ the moment of force and I the moment of inertia.
- Torsion pendulum: $T = 2\pi\sqrt{I/\kappa}$ with $\kappa = \dfrac{2lm}{\pi r^4 \Delta\varphi}$ the constant of torsion and I the moment of inertia.
- Mathematic pendulum: $T = 2\pi\sqrt{l/g}$ with g the acceleration of gravity and l the length of the pendulum.

Chapter 5

Waves

5.1 The wave equation

The general shape of the wave equation is: $\square u = 0$, or:

$$\nabla^2 u - \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} - \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} = 0$$

where u is the disturbance and v the *propagation velocity*. In general holds: $v = f\lambda$. Per definition holds: $k\lambda = 2\pi$ and $\omega = 2\pi f$.

In principle, there are two kinds of waves:

1. Longitudinal waves: for these holds $\vec{k} \parallel \vec{v} \parallel \vec{u}$.
2. Transversal waves: for these holds $\vec{k} \parallel \vec{v} \perp \vec{u}$.

The *phase velocity* is given by $v_{\rm ph} = \omega/k$. The *group velocity* is given by:

$$v_{\rm g} = \frac{d\omega}{dk} = v_{\rm ph} + f\frac{dv_{\rm ph}}{dk} = v_{\rm ph}\left(1 - \frac{k}{n}\frac{dn}{dk}\right)$$

where n is the refractive index of the medium. If one want to transfer information with a wave, e.g. by modulating it, will the information move with the group velocity. If $v_{\rm ph}$ does not depend on ω holds: $v_{\rm ph} = v_{\rm g}$. In a dispersive medium it is possible that $v_{\rm g} > v_{\rm ph}$ or $v_{\rm g} < v_{\rm ph}$.
For some media, the propagation velocity follows from:

- Pressure waves in a liquid or gas: $v = \sqrt{\kappa/\varrho}$, where κ is the modulus of compression.
- For pressure waves in a gas also holds: $v = \sqrt{\gamma p/\varrho} = \sqrt{\gamma RT/M}$.
- Pressure waves in a solid bar: $v = \sqrt{E/\varrho}$
- waves in a string: $v = \sqrt{F_{\rm span} l/m}$
- Surface waves on a liquid: $v = \sqrt{\left(\frac{g\lambda}{2\pi} + \frac{2\pi\gamma}{\varrho\lambda}\right)\tanh\left(\frac{2\pi h}{\lambda}\right)}$
  where h is the depth of the liquid and γ the surface tension. If $h \ll \lambda$ holds: $v \approx \sqrt{gh}$.

5.2 Solutions of the wave equation

5.2.1 Plane waves

In n dimensions a harmonic plane wave is defined by:

$$u(\vec{x}, t) = 2^n \hat{u}\cos(\omega t)\sum_{i=1}^{n}\sin(k_i x_i)$$

The equation for a harmonic traveling plane wave is: $u(\vec{x}, t) = \hat{u}\cos(\vec{k}\cdot\vec{x} \pm \omega t + \varphi)$

If waves reflect at the end of a spring will this result in a change in phase. A fixed end gives a phase change of $\pi/2$ to the reflected wave, with boundary condition $u(l) = 0$. A lose end gives no change in the phase of the reflected wave, with boundary condition $(\partial u/\partial x)_l = 0$.

If an observer is moving w.r.t. the wave with a velocity $v_{\rm obs}$, he will observe a change in frequency: the *Doppler effect*. This is given by: $\dfrac{f}{f_0} = \dfrac{v_{\rm f} - v_{\rm obs}}{v_{\rm f}}$.

5.2.2 Spherical waves

When the situation is spherical symmetric, the homogeneous wave equation is given by:

$$\frac{1}{v^2}\frac{\partial^2(ru)}{\partial t^2} - \frac{\partial^2(ru)}{\partial r^2} = 0$$

with general solution:

$$u(r,t) = C_1\frac{f(r-vt)}{r} + C_2\frac{g(r+vt)}{r}$$

5.2.3 Cylindrical waves

When the situation has a cylindrical symmetry, the homogeneous wave equation becomes:

$$\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2} - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = 0$$

This is a Bessel equation, with solutions which can be written as Hankel functions. For sufficient large values of r these are approximated with:

$$u(r,t) = \frac{\hat{u}}{\sqrt{r}}\cos(k(r \pm vt))$$

5.2.4 The general solution in one dimension

Starting point is the equation:

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \sum_{m=0}^{N}\left(b_m\frac{\partial^m}{\partial x^m}\right)u(x,t)$$

where $b_m \in I\!\!R$. Substituting $u(x,t) = A{\rm e}^{i(kx-\omega t)}$ gives two solutions $\omega_j = \omega_j(k)$ as dispersion relations. The general solution is given by:

$$u(x,t) = \int\limits_{-\infty}^{\infty}\left(a(k){\rm e}^{i(kx-\omega_1(k)t)} + b(k){\rm e}^{i(kx-\omega_2(k)t)}\right)dk$$

Because in general the frequencies ω_j are non-linear in k there is dispersion and the solution can not be written any more as a sum of functions depending only on $x \pm vt$: the wave front transforms.

5.3 The stationary phase method

The Fourier integrals of the previous section can usually not be calculated exact. If $\omega_j(k) \in I\!\!R$ the stationary phase method can be applied. Assuming that $a(k)$ is only a slowly varying function of k, one can state that the parts of the k-axis where the phase of $kx-\omega(k)t$ changes rapidly will give no net contribution to the integral because the exponent oscillates rapidly there. The only areas contributing significantly to the integral are areas with a stationary phase, determined by $\dfrac{d}{dk}(kx - \omega(k)t) = 0$. Now the following approximation is possible:

$$\int\limits_{-\infty}^{\infty} a(k){\rm e}^{i(kx-\omega(k)t)}dk \approx \sum_{i=1}^{N}\sqrt{\frac{2\pi}{\frac{d^2\omega(k_i)}{dk_i^2}}}\exp\left[-i\tfrac{1}{4}\pi + i(k_i x - \omega(k_i)t)\right]$$

5.4 Green functions for the initial-value problem

This method is preferable if the solutions deviate much from the stationary solutions, like point-like excitations. Starting with the wave equation in one dimension, with $\nabla^2=\partial^2/\partial x^2$ holds: if $Q(x,x',t)$ is the solution with initial values $Q(x,x',0)=\delta(x-x')$ and $\dfrac{\partial Q(x,x',0)}{\partial t}=0$, and $P(x,x',t)$ the solution with initial values $P(x,x',0)=0$ and $\dfrac{\partial P(x,x',0)}{\partial t}=\delta(x-x')$, then the solution of the wave equation with arbitrary initial conditions $f(x)=u(x,0)$ and $g(x)=\dfrac{\partial u(x,0)}{\partial t}$ is given by:

$$u(x,t)=\int\limits_{-\infty}^{\infty}f(x')Q(x,x',t)dx'+\int\limits_{-\infty}^{\infty}g(x')P(x,x',t)dx'$$

P and Q are called the *propagators*. They are defined by: door:

$$\begin{array}{rcl}Q(x,x',t)&=&\frac{1}{2}[\delta(x-x'-vt)+\delta(x-x'+vt)]\\ P(x,x',t)&=&\left\{\begin{array}{ll}\dfrac{1}{2v}&\text{if }\ |x-x'|<vt\\ 0&\text{if }\ |x-x'|>vt\end{array}\right.\end{array}$$

Further holds the relation: $Q(x,x',t)=\dfrac{\partial P(x,x',t)}{\partial t}$

5.5 Waveguides and resonating cavities

The boundary conditions at a perfect conductor can be derived from the Maxwell equations. If $\vec{n}$ is a unit vector ⊥ the surface, aimed from 1 to 2, and $\vec{K}$ is a surface current density, than holds:

$$\begin{array}{ll}\vec{n}\cdot(\vec{D}_2-\vec{D}_1)=\sigma & \vec{n}\times(\vec{E}_2-\vec{E}_1)=0\\ \vec{n}\cdot(\vec{B}_2-\vec{B}_1)=0 & \vec{n}\times(\vec{H}_2-\vec{H}_1)=\vec{K}\end{array}$$

In a waveguide holds because of the cylindrical symmetry: $\vec{E}(\vec{x},t)=\vec{\mathcal{E}}(x,y)\mathrm{e}^{i(kz-\omega t)}$ and $\vec{B}(\vec{x},t)=\vec{\mathcal{B}}(x,y)\mathrm{e}^{i(kz-\omega t)}$. One can now deduce that, if $\mathcal{B}_z$ and $\mathcal{E}_z$ are not $\equiv 0$:

$$\begin{array}{ll}\mathcal{B}_x=\dfrac{i}{\varepsilon\mu\omega^2-k^2}\left(k\dfrac{\partial\mathcal{B}_z}{\partial x}-\varepsilon\mu\omega\dfrac{\partial\mathcal{E}_z}{\partial y}\right) & \mathcal{B}_y=\dfrac{i}{\varepsilon\mu\omega^2-k^2}\left(k\dfrac{\partial\mathcal{B}_z}{\partial y}+\varepsilon\mu\omega\dfrac{\partial\mathcal{E}_z}{\partial x}\right)\\ \mathcal{E}_x=\dfrac{i}{\varepsilon\mu\omega^2-k^2}\left(k\dfrac{\partial\mathcal{E}_z}{\partial x}+\varepsilon\mu\omega\dfrac{\partial\mathcal{B}_z}{\partial y}\right) & \mathcal{E}_y=\dfrac{i}{\varepsilon\mu\omega^2-k^2}\left(k\dfrac{\partial\mathcal{E}_z}{\partial y}-\varepsilon\mu\omega\dfrac{\partial\mathcal{B}_z}{\partial x}\right)\end{array}$$

Now one can distinguish between three cases:

1. $B_z\equiv 0$: the Transversal Magnetic modes (TM). Boundary condition: $\mathcal{E}_z|_{\rm surf}=0$.
2. $E_z\equiv 0$: the Transversal Electric modes (TE). Boundary condition: $\left.\dfrac{\partial\mathcal{B}_z}{\partial n}\right|_{\rm surf}=0$.

   For the TE and TM modes this gives an eigenvalue problem for $\mathcal{E}_z$ resp. $\mathcal{B}_z$ with as boundary conditions:

   $$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi=-\gamma^2\psi\ \text{ with eigenvalues }\ \gamma^2:=\varepsilon\mu\omega^2-k^2$$

   This gives a discrete solution ψ_ℓ at eigenvalue γ_ℓ^2: $k=\sqrt{\varepsilon\mu\omega^2-\gamma_\ell^2}$. For $\omega<\omega_\ell$, k is imaginary and the wave is damped. Therefore, ω_ℓ is called the *cut-off frequency*. In rectangular conductors the following expression can be found for the cut-off frequency for modes $\mathrm{TE}_{m,n}$ of $\mathrm{TM}_{m,n}$:

   $$\lambda_\ell=\frac{2}{\sqrt{(m/a)^2+(n/b)^2}}$$

3. E_z and B_z are zero everywhere: the Transversal electromagnetic mode (TEM). Than holds: $k = \pm\omega\sqrt{\varepsilon\mu}$ and $v_{\rm f} = v_{\rm g}$, just as if here were no waveguide. Further $k \in I\!R$, so there exist no cut-off frequency.

In a rectangular, 3 dimensional resonating cavity with edges a, b and c are the possible wave numbers given by: $k_x = \dfrac{n_1\pi}{a}$, $k_y = \dfrac{n_2\pi}{b}$, $k_z = \dfrac{n_3\pi}{c}$ This results in the possible frequencies $f = vk/2\pi$ in the cavity:

$$f = \frac{v}{2}\sqrt{\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}}$$

For a cubic cavity, with $a = b = c$, the possible number of oscillating modes $N_{\rm L}$ for longitudinal waves is given by:

$$N_{\rm L} = \frac{4\pi a^3 f^3}{3v^3}$$

Because transversal waves have two possible polarizations holds for them: $N_{\rm T} = 2N_{\rm L}$.

5.6 Non-linear wave equations

The *Van der Pol* equation is given by:

$$\frac{d^2x}{dt^2} - \varepsilon\omega_0(1 - \beta x^2)\frac{dx}{dt} + \omega_0^2 x = 0$$

βx^2 can be ignored for very small values of the amplitude. Substitution of $x \sim {\rm e}^{i\omega t}$ gives: $\omega = \frac{1}{2}\omega_0(i\varepsilon \pm 2\sqrt{1 - \frac{1}{2}\varepsilon^2})$. The lowest-order instabilities grow with $\frac{1}{2}\varepsilon\omega_0$. While x is growing, the 2nd term becomes larger and decreases the growth. Oscillations on a time scale $\sim \omega_0^{-1}$ can exist. If x is developed as $x = x^{(0)} + \varepsilon x^{(1)} + \varepsilon^2 x^{(2)} + \cdots$ and this is substituted we have, besides periodic, *secular terms* $\sim \varepsilon t$. If we assume there exist some timescales τ_n, $0 \leq \tau \leq N$ with $\partial\tau_n/\partial t = \varepsilon^n$ and if we put the secular terms 0 we get:

$$\frac{d}{dt}\left\{\frac{1}{2}\left(\frac{dx}{dt}\right)^2 + \tfrac{1}{2}\omega_0^2 x^2\right\} = \varepsilon\omega_0(1 - \beta x^2)\left(\frac{dx}{dt}\right)^2$$

This is an energy equation. Energy is conserved if the left-hand side is 0. If $x^2 > 1/\beta$, the right-hand side changes sign and an increase in energy changes into a decrease of energy. This mechanism limits the growth of oscillations.

The *Korteweg-De Vries* equation is given by:

$$\frac{\partial u}{\partial t} + \underbrace{au\frac{\partial u}{\partial x}}_{\rm non-lin} + \underbrace{b\frac{\partial^3 u}{\partial x^3}}_{\rm dispersive} = 0$$

This equation is for example a model for ion-acoustic waves in a plasma. For this equation, soliton solutions of the following shape exist:

$$u(x - ct) = \frac{3c}{\cosh^2(\frac{1}{2}\sqrt{2}(x - ct))}$$

Chapter 6

Optics

6.1 The bending of light

For the refraction at a surface holds: $n_i \sin(\theta_i) = n_t \sin(\theta_t)$ where n is the *refractive index* of the material. Snell's law is:

$$\frac{n_2}{n_1} = \frac{\lambda_1}{\lambda_2} = \frac{v_1}{v_2}$$

If $\Delta n \leq 1$, the change in phase of the light is $\Delta\varphi = 0$, if $\Delta n > 1$ holds: $\Delta\varphi = \pi$. The refraction of light in a material is caused by scattering at atoms. This is described by:

$$n^2 = 1 + \frac{n_{\rm e} e^2}{\varepsilon_0 m} \sum_j \frac{f_j}{\omega_{0,j}^2 - \omega^2 - i\delta\omega}$$

where $n_{\rm e}$ is the electron density and f_j the *oscillator strength*, for which holds: $\sum\limits_j f_j = 1$. From this follows that $v_{\rm g} = c/(1 + (n_{\rm e} e^2 / 2\varepsilon_0 m\omega^2))$. From this the equation of Cauchy can be derived: $n = a_0 + a_1/\lambda^2$. More general, it is possible to develop n as: $n = \sum\limits_{k=0}^{n} \frac{a_k}{\lambda^{2k}}$.

For an electromagnetic wave in general holds: $n = \sqrt{\varepsilon_{\rm r} \mu_{\rm r}}$.

The path, followed by a lightray in material can be found with *Fermat's principle*:

$$\delta \int_1^2 dt = \delta \int_1^2 \frac{n(s)}{c} ds = 0 \Rightarrow \delta \int_1^2 n(s) ds = 0$$

6.2 Paraxial geometrical optics

6.2.1 Lenses

The Gaussian lens formula can be deduced from Fermat's principle with the approximations $\cos\varphi = 1$ and $\sin\varphi = \varphi$. For the refraction at a spherical surface with radius R holds:

$$\frac{n_1}{v} - \frac{n_2}{b} = \frac{n_1 - n_2}{R}$$

where $|v|$ is the distance of the object and $|b|$ the distance of the image. Applying this twice results in:

$$\frac{1}{f} = (n_{\rm l} - 1)\left(\frac{1}{R_2} - \frac{1}{R_1}\right)$$

where $n_{\rm l}$ is the refractive index of the lens, f is the focal length and R_1 and R_2 are the curvature radii of both surfaces. For a double concave lens holds $R_1 < 0$, $R_2 > 0$, for a double convex lens holds $R_1 > 0$ and $R_2 < 0$. Further holds:

$$\frac{1}{f} = \frac{1}{v} - \frac{1}{b}$$

$D := 1/f$ is called the dioptric power of a lens. For a lens with thickness d and diameter D holds in good approximation: $1/f = 8(n-1)d/D^2$. For two lenses placed on a line with distance d holds:

$$\frac{1}{f} = \frac{1}{f_1} + \frac{1}{f_2} - \frac{d}{f_1 f_2}$$

In these equations the following signs are being used for refraction at a spherical surface, as is seen by an incoming lightray:

Quantity	+	−
R	Concave surface	Convex surface
f	Converging lens	Diverging lens
v	Real object	Virtual object
b	Virtual image	Real image

6.2.2 Mirrors

For images of mirrors holds:

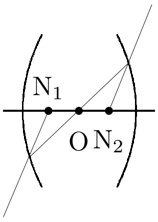
$$\frac{1}{f}=\frac{1}{v}+\frac{1}{b}=\frac{2}{R}+\frac{h^2}{2}\left(\frac{1}{R}-\frac{1}{v}\right)^2$$

where h is the perpendicular distance from the point the light ray hits the mirror to the optical axis. Spherical aberration can be reduced by not using spherical mirrors. A parabolical mirror has no spherical aberration for light rays parallel with the optical axis and is therefore often used for telescopes. The used signs are:

Quantity	+	−
R	Concave mirror	Convex mirror
f	Concave mirror	Convex mirror
v	Real object	Virtual object
b	Real image	Virtual image

6.2.3 Principal planes

The *nodal points* N of a lens are defined by the figure on the right. If the lens is surrounded by the same medium on both sides, the nodal points are the same as the principal points H. The plane ⊥ the optical axis through the principal points is called the *principal plane*. Is the lens is described by a matrix m_{ij} holds for the distances h_1 and h_2 to the boundary of the lens:



$$h_1=n\frac{m_{11}-1}{m_{12}}\quad,\quad h_2=n\frac{m_{22}-1}{m_{12}}$$

6.2.4 Magnification

The *linear magnification* is defined by: $N=-\frac{b}{v}$

The *angular magnification* is defined by: $N_\alpha=-\frac{\alpha_{\rm syst}}{\alpha_{\rm none}}$

where $\alpha_{\rm sys}$ is size of the retinal image with the optical system and $\alpha_{\rm none}$ the size of the retinal image without the system. Further holds: $N\cdot N_\alpha=1$. For a telescope holds: $N=f_{\rm objective}/f_{\rm ocular}$. The *f-number* is defined by $f/D_{\rm objective}$.

6.3 Matrix methods

A light ray can be described by a vector $(n\alpha,y)$ with α the angle with the optical axis and y the distance to the optical axis. The change of a light ray interacting with an optical system can be obtained using a matrix multiplication:

$$\begin{pmatrix} n_2\alpha_2 \\ y_2 \end{pmatrix}=M\begin{pmatrix} n_1\alpha_1 \\ y_1 \end{pmatrix}$$

where $\mathrm{Tr}(M)=1$. M is a product of elementary matrices. These are:

1. Transfer along length l: $M_{\rm R} = \begin{pmatrix} 1 & 0 \\ l/n & 1 \end{pmatrix}$
2. Refraction at a surface with dioptric power D: $M_{\rm T} = \begin{pmatrix} 1 & -D \\ 0 & 1 \end{pmatrix}$

6.4 Aberrations

Lenses usually do not give a perfect image. Some causes are:

1. **Chromatic aberration** is caused by the fact that $n = n(\lambda)$. This can be partially corrected with a lens which is composed of more lenses with different functions $n_i(\lambda)$. Using N lenses makes it possible to obtain the same f for N wavelengths.
2. **Spherical aberration** is caused by second-order effects which are usually ignored; a spherical surface does not make a perfect lens. Incomming rays far from the optical axis will more bent.
3. **Coma** is caused by the fact that the principal planes of a lens are only plane near the principal axis. Further away of the optical axis they are curved. This curvature can be both positive or negative.
4. **Astigmatism**: from each point of an object not on the optical axis the image is an ellipse because the thickness of the lens is not the same everywhere.
5. **Field curvature** can be corrected by the human eye.
6. **Distorsion** gives abberations near the borders of the image. This can be corrected with a combination of positive and negative lenses.

6.5 Reflection and transmission

If an electromagnetic wave hits a transparent medium a part of the wave shall reflect at the same angle as the incident angle, and a part will be refracted at an angle following from Snell's law. It makes a difference whether the $\vec{E}$ field of the wave is ⊥ or ∥ w.r.t. the surface. When the coefficients of reflection r and transmission t are defined as:

$$r_{\parallel} \equiv \left(\frac{E_{0r}}{E_{0i}}\right)_{\parallel} ~,~~ r_{\perp} \equiv \left(\frac{E_{0r}}{E_{0i}}\right)_{\perp} ~,~~ t_{\parallel} \equiv \left(\frac{E_{0t}}{E_{0i}}\right)_{\parallel} ~,~~ t_{\perp} \equiv \left(\frac{E_{0t}}{E_{0i}}\right)_{\perp}$$

where E_{0r} is the reflected amplitude and E_{0t} the transmitted amplitude. Then the Fresnel equations are:

$$r_{\parallel} = \frac{\tan(\theta_i - \theta_t)}{\tan(\theta_i + \theta_t)} ~~,~~ r_{\perp} = \frac{\sin(\theta_t - \theta_i)}{\sin(\theta_t + \theta_i)}$$

$$t_{\parallel} = \frac{2\sin(\theta_t)\cos(\theta_i)}{\sin(\theta_t + \theta_i)\cos(\theta_t - \theta_i)} ~~,~~ t_{\perp} = \frac{2\sin(\theta_t)\cos(\theta_i)}{\sin(\theta_t + \theta_i)}$$

The following holds: $t_{\perp} - r_{\perp} = 1$ and $t_{\parallel} + r_{\parallel} = 1$. If the coefficient of reflection R and transmission T are defined as (with $\theta_i = \theta_r$):

$$R \equiv \frac{I_r}{I_i} \quad \text{and} \quad T \equiv \frac{I_t\cos(\theta_t)}{I_i\cos(\theta_i)}$$

with $I = \langle|\vec{S}|\rangle$ follows: $R + T = 1$. Special is the case $r_{\perp} = 0$. This happens if the angle between the reflected and transmitted rays is 90°. From Snell's law then follows: $\tan(\theta_i) = n$. This angle is called *Brewster's angle*. The situation with $r_{\parallel} = 0$ is not possible.

6.6 Polarization

The polarization is defined as: $P = \dfrac{I_{\rm p}}{I_{\rm p}+I_{\rm u}} = \dfrac{I_{\rm max}-I_{\rm min}}{I_{\rm max}+I_{\rm min}}$

where the intensity of the polarized light is given by $I_{\rm p}$ and the intensity of the unpolarized light is given by $I_{\rm u}$. $I_{\rm max}$ and $I_{\rm min}$ are the maximum and minimum intensities when the light passes a polarizer. If polarized light passes through a polarizer *Malus law* applies: $I(\theta) = I(0)\cos^2(\theta)$ where θ is the angle of the polarizer.

The state of a light ray can be described with the *Stokes-parameters*: start with 4 filters which each let pass half the intensity. The first is independent of the polarization, the second and third are linear polarizers with the transmission axes horizontal and at +45°, while the fourth is a circular polarizer which is opaque for L-states. Then holds $S_1 = 2I_1$, $S_2 = 2I_2 - 2I_1$, $S_3 = 2I_3 - 2I_1$ and $S_4 = 2I_4 - 2I_1$.

The state of a *polarized* light ray can also be described with the *Jones vector*:

$$\vec{E} = \left(\begin{array}{c} E_{0x}{\rm e}^{i\varphi_x} \\ E_{0y}{\rm e}^{i\varphi_y} \end{array} \right)$$

For the horizontal P-state holds: $\vec{E} = (1,0)$, for the vertical P-state $\vec{E} = (0,1)$, the R-state is given by $\vec{E} = \frac{1}{2}\sqrt{2}(1,-i)$ and the L-state by $\vec{E} = \frac{1}{2}\sqrt{2}(1,i)$. The change in state of a light beam after passage of optical equipment can be described as $\vec{E}_2 = M \cdot \vec{E}_1$. For some kinds of optical equipment the Jones matrix M is given by:

Horizontal linear polarizer:	$\left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right)$
Vertical linear polarizer:	$\left(\begin{array}{cc} 0 & 0 \\ 0 & 1 \end{array}\right)$
Linear polarizer at +45°	$\frac{1}{2}\left(\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array}\right)$
Lineair polarizer at −45°	$\frac{1}{2}\left(\begin{array}{cc} 1 & -1 \\ -1 & 1 \end{array}\right)$
$\frac{1}{4}$-λ plate, fast axis vertical	${\rm e}^{i\pi/4}\left(\begin{array}{cc} 1 & 0 \\ 0 & -i \end{array}\right)$
$\frac{1}{4}$-λ plate, fast axis horizontal	${\rm e}^{i\pi/4}\left(\begin{array}{cc} 1 & 0 \\ 0 & i \end{array}\right)$
Homogene circulair polarizor right	$\frac{1}{2}\left(\begin{array}{cc} 1 & i \\ -i & 1 \end{array}\right)$
Homogene circular polarizer left	$\frac{1}{2}\left(\begin{array}{cc} 1 & -i \\ i & 1 \end{array}\right)$

6.7 Prisms and dispersion

A light ray passing through a prism is refracted twice and gets a deviation from it's original direction $\delta = \theta_i + \theta_{i'} + \alpha$ w.r.t. the incident direction, where α is the apex angle, θ_i is the angle between the incident angle and a line perpendicular to the surface and $\theta_{i'}$ is the angle between the ray leaving the prism and a line perpendicular to the surface. When θ_i varies there is an angle for which δ becomes minimal. For the refractive index of the prism now holds:

$$n = \frac{\sin(\frac{1}{2}(\delta_{\rm min} + \alpha))}{\sin(\frac{1}{2}\alpha)}$$

The dispersion of a prism is defined by:

$$D = \frac{d\delta}{d\lambda} = \frac{d\delta}{dn}\frac{dn}{d\lambda}$$

where the first factor depends on the shape and the second on the composition of the prism. For the first factor follows:

$$\frac{d\delta}{dn}=\frac{2\sin(\frac{1}{2}\alpha)}{\cos(\frac{1}{2}(\delta_{\rm min}+\alpha))}$$

For visible light usually holds $dn/d\lambda < 0$: shorter wavelengths are stronger bent than longer. The refractive index in this area can usually be approximated by Cauchy's formula.

6.8 Diffraction

Fraunhofer diffraction occurs far away of the source(s). The Fraunhofer diffraction of light passing through multiple slits is described by:

$$\frac{I(\theta)}{I_0}=\left(\frac{\sin(u)}{u}\right)^2\cdot\left(\frac{\sin(Nv)}{\sin(v)}\right)^2$$

where $u=\pi b\sin(\theta)/\lambda$, $v=\pi d\sin(\theta)/\lambda$. N is the number of slits, b is the width of a slit and d is the distance between the slits. The maxima in intensity are given by $d\sin(\theta)=k\lambda$.

The diffraction through a spherical aperture with radius a is described by:

$$\frac{I(\theta)}{I_0}=\left(\frac{J_1(ka\sin(\theta))}{ka\sin(\theta)}\right)^2$$

The diffraction pattern of a rectangular aperture at distance R with length a in the x-direction and b in the y-direction is described by:

$$\frac{I(x,y)}{I_0}=\left(\frac{\sin(\alpha')}{\alpha'}\right)^2\left(\frac{\sin(\beta')}{\beta'}\right)^2$$

where $\alpha'=kax/2R$ and $\beta'=kby/2R$.

When X rays are diffracted at a crystal holds for the position of the maxima in intensity *Bragg's relation*: $2d\sin(\theta)=n\lambda$ where d is the distance between the crystal layers.

Close at the source the Fraunhofermodel is unusable because it ignores the angle-dependence of the reflected waves. This is described by the *obliquity* or *inclination factor*, which describes the directionality of the secondary emissions: $E(\theta)=\frac{1}{2}E_0(1+\cos(\theta))$ where θ is the angle with the optical axis.

Diffraction limits the *resolution* of a system. This is the minimum angle $\Delta\theta_{\rm min}$ between two incident rays coming from points far away for which their refraction patterns can be detected separately. For a circular slit holds: $\Delta\theta_{\rm min}=1,22\lambda/D$ where D is the diameter of the slit.

For a grating holds: $\Delta\theta_{\rm min}=2\lambda/(Na\cos(\theta_m))$ where a is the distance between two peaks and N the number of peaks. The minimum difference between two wavelengths that gives a separated diffraction pattern in a multiple slit geometry is given by $\Delta\lambda/\lambda=nN$ where N is the number of lines and n the order of the pattern.

6.9 Special optical effects

- **Birefringe and dichroism**. $\vec{D}$ is not parallel with $\vec{E}$ if the polarizability $\vec{P}$ of a material is nut equal in all directions. There are at least 3 directions, the *principal axes*, in which they are parallel. This results in 3 refractive indices n_i with can be used to construct Fresnel's ellipsoid. In case $n_2=n_3\neq n_1$, which happens e.g. at trigonal, hexagonal and tetragonal crystals there is one optical axis in the direction of n_1. Incident light rays can now be split up in two parts: the *ordinary wave* is linear polarized $\perp$ the plane through the transmission direction and the optical axis. The *extraordinary wave* is linear polarized in the plane through the transmission direction and the optical axis. *Dichroism* is caused by a different absorption of the ordinary and extraordinary wave in some materials. *Double images* occur when the incident ray makes an angle with optical axis: the extraordinary wave will refract, the ordinary will not.

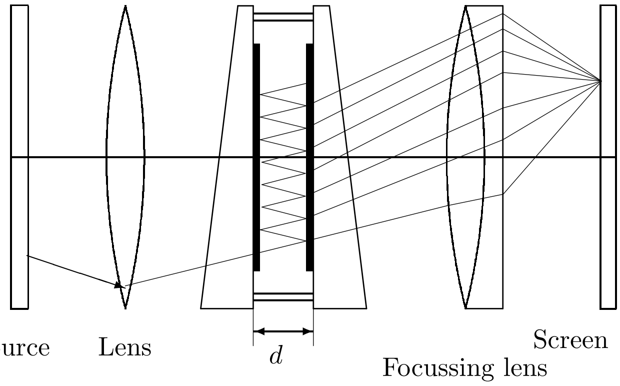
- **Retarders: waveplates and compensators**. Incident light will have a phase shift of $\Delta\varphi = 2\pi d(|n_0 - n_{\rm e}|)/\lambda_0$ if an uniaxial crystal is cut in such a way that the optical axis is parallel with the front and back plane. Here, λ_0 is the wavelength in vacuum and n_0 and $n_{\rm e}$ the refractive indices for the ordinary and extraordinary wave. For a quarter-wave plate holds: $\Delta\varphi = \pi/2$.
- **The Kerr-effect**: isotropic, transparent materials can become birefringent when placed in an electric field. In that case, the optical axis is parallel to $\vec{E}$. The difference in refractive index in the two directions is given by: $\Delta n = \lambda_0 K E^2$, where K is the *Kerr constant* of the material. If the electrodes have an effective length ℓ and are separated by a distance d, the retardation is given by: $\Delta\varphi = 2\pi K\ell V^2/d^2$, where V is the applied voltage.
- **The Pockels** or linear electro-optical effect can occur in 20 (from a total of 32) crystal symmetry classes, namely those without a center of symmetry. These crystals are also *piezoelectric*: their polarization changes when a pressure is applied and vice versa: $\vec{P} = pd + \varepsilon_0\chi\vec{E}$. The retardation in a Pockels cell is $\Delta\varphi = 2\pi n_0^3 r_{63} V/\lambda_0$ where r_{63} is the 6-3 element of the electro-optic tensor.
- **The Faraday effect**: the polarization of light passing through material with length d and on which a magnetic field is applied in the propagation direction is rotated by an angle $\beta = \mathcal{V}Bd$ where $\mathcal{V}$ is the *Verdet constant.*
- **Čerenkov radiation** arises when a particle with arrives with $v_q > v_{\rm f}$. The radiation is emitted within a cone with an apex angle α with $\sin(\alpha) = c/c_{\rm medium} = c/nv_q$.

6.10 The Fabry-Perot interferometer

For a Fabry-Perot interferometer holds in general: $T + R + A = 1$ where T is the transmission factor, R the reflection factor and A the absorption factor. If F is given by $F = 4R/(1-R)^2$ follows for the intensity distribution:

$$\frac{I_t}{I_i} = \left[1 - \frac{A}{1-R}\right]^2 \frac{1}{1 + F\sin^2(\theta)}$$

The term $[1 + F\sin^2(\theta)]^{-1} := \mathcal{A}(\theta)$ is called the *Airy function.*



The width of the peaks at half height is given bt $\gamma = 4/\sqrt{F}$. The *finesse* $\mathcal{F}$ is defined as $\mathcal{F} = \frac{1}{2}\pi\sqrt{F}$. The maximum resolution is then given by $\Delta f_{\rm min} = c/2nd\mathcal{F}$.

Chapter 7

Statistical physics

7.1 Degrees of freedom

A molecule consisting of n atoms has $s = 3n$ degrees of freedom. There are 3 translational degrees of freedom, a linear molecule has $s = 3n - 5$ vibrational degrees of freedom and a non-linear molecule $s = 3n - 6$. A linear molecule has 2 rotational degrees of freedom and a non-linear molecule 3.

Because vibrational degrees of freedom account for both kinetic and potential energy they count double. So, for linear molecules this results in a total of $s = 6n - 5$. For non-linear molecules this gives $s = 6n - 6$. The average energy of a molecule in thermodynamic equilibrium is $\langle E_{\rm tot}\rangle = \frac{1}{2}skT$. Each degree of freedom of a molecule has in principle the same energy: the *principle of equipartition.*

The rotational and vibrational energy of a molecule are:

$$W_{\rm rot} = \frac{\hbar^2}{2I}l(l+1) = Bl(l+1)\ ,\quad W_{\rm vib} = (v + \tfrac{1}{2})\hbar\omega_0$$

The vibrational levels are excited if $kT \approx \hbar\omega$, the rotational levels of a hetronuclear molecule are excited if $kT \approx 2B$. For homonuclear molecules additional selection rules apply so the rotational levels are well coupled if $kT \approx 6B$.

7.2 The energy distribution function

The general shape of the equilibrium velocity distribution function is
$P(v_x, v_y, v_z)dv_xdv_ydv_z = P(v_x)dv_x \cdot P(v_y)dv_y \cdot P(v_z)dv_z$ with

$$P(v_i)dv_i = \frac{1}{\alpha\sqrt{\pi}}\exp\left(-\frac{v_i^2}{\alpha^2}\right)dv_i$$

where $\alpha = \sqrt{2kT/m}$ is the *most probable velocity* of a particle. The average velocity is given by $\langle v\rangle = 2\alpha/\sqrt{\pi}$, and $\langle v^2\rangle = \frac{3}{2}\alpha^2$. The distribution as a function of the absolute value of the velocity is given by:

$$\frac{dN}{dv} = \frac{4N}{\alpha^3\sqrt{\pi}}\,v^2\exp\left(-\frac{mv^2}{2kT}\right)$$

The general shape of the energy distribution function then becomes:

$$P(E)dE = \frac{c(s)}{kT}\left(\frac{E}{kT}\right)^{\frac{1}{2}s-1}\exp\left(-\frac{E}{kT}\right)$$

where $c(s)$ is a normalization constant, given by:

1. Even s: $s = 2l$: $c(s) = \dfrac{1}{(l-1)!}$
2. Odd s: $s = 2l+1$: $c(s) = \dfrac{2^l}{\sqrt{\pi}(2l-1)!!}$

7.3 Pressure on a wall

The number of molecules that collides with a wall with surface A within a time τ is given by:

$$\iiint d^3N = \int\limits_0^\infty \int\limits_0^\pi \int\limits_0^{2\pi} nAv\tau\cos(\theta)P(v,\theta,\varphi)dvd\theta d\varphi$$

From this follows for the particle flux on the wall: $\Phi = \frac{1}{4}n\langle v\rangle$. For the pressure on the wall then follows:

$$d^3p = \frac{2mv\cos(\theta)d^3N}{A\tau}\ ,\quad \text{so}\quad p = \frac{2}{3}n\langle E\rangle$$

7.4 The equation of state

If intermolecular forces and the own volume of the molecules can be neglected can for gases from $p = \frac{2}{3}n\langle E\rangle$ and $\langle E\rangle = \frac{3}{2}kT$ be derived:

$$pV = n_sRT = \frac{1}{3}Nm\left\langle v^2\right\rangle$$

Here, n_s is the number of *moles* particles and N is the total number of particles within volume V. If the own volume and the intermolecular forces can not be neglected the *Van der Waals* equation can be derived:

$$\left(p + \frac{an_s^2}{V^2}\right)(V - bn_s) = n_sRT$$

There is an isotherme with a horizontal point of inflection. In the Van der Waals equation this corresponds with the *critical temperature, pressure* and *volume* of the gas. This is the upper limit of the area of coexistence between liquid and vapor. From $dp/dV = 0$ and $d^2p/dV^2 = 0$ follows:

$$T_{\rm cr} = \frac{8a}{27bR}\ ,\quad p_{\rm cr} = \frac{a}{27b^2}\ ,\quad V_{\rm cr} = 3bn_s$$

For the critical point holds: $p_{\rm cr}V_{m,{\rm cr}}/RT_{\rm cr} = \frac{3}{8}$, which differs from the value of 1 which follows from the general gas law.

Scaled on the critical quantities, with $p^* := p/p_{\rm cr}$, $T^* = T/T_{\rm cr}$ and $V_m^* = V_m/V_{m,{\rm cr}}$ with $V_m := V/n_s$ holds:

$$\left(p^* + \frac{3}{(V_m^*)^2}\right)(V_m^* - \tfrac{1}{3}) = \tfrac{8}{3}T^*$$

Gases behave the same for equal values of the reduced quantities: the *law of the corresponding states.* A *virial development* is used for even more accurate contemplations:

$$p(T, V_m) = RT\left(\frac{1}{V_m} + \frac{B(T)}{V_m^2} + \frac{C(T)}{V_m^3} + \cdots\right)$$

The *Boyle temperature* $T_{\rm B}$ is the temperature for which the 2nd virial coefficient is 0. In a Van der Waals gas, this happens at $T_{\rm B} = a/Rb$. The *inversion temperature* $T_{\rm i} = 2T_{\rm B}$.

The equation of state for solids and liquids is given by:

$$\frac{V}{V_0} = 1 + \gamma_p\Delta T - \kappa_T\Delta p = 1 + \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p\Delta T + \frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T\Delta p$$

7.5 Collisions between molecules

The collision probability of a particle in a gas that is translated over a distance dx is given bt $n\sigma dx$, where σ is the *cross section*. The mean free path is given by $\ell = \frac{v_1}{nu\sigma}$ with $u = \sqrt{v_1^2 + v_2^2}$ the relative velocity between the particles. If $m_1 \ll m_2$ holds: $\frac{u}{v_1} = \sqrt{1 + \frac{m_1}{m_2}}$, so $\ell = \frac{1}{n\sigma}$. If $m_1 = m_2$ holds: $\ell = \frac{1}{n\sigma\sqrt{2}}$. This means that the average time between two collisions is given by $\tau = \frac{1}{n\sigma v}$. If the molecules are approximated with hard spheres the cross section is: $\sigma = \frac{1}{4}\pi(D_1^2 + D_2^2)$. The average distance between two molecules is $0,55n^{-1/3}$. Collisions between molecules and small particles in a solution result in the *Brownian motion*. For the average motion of a particle with radius R can be derived: $\langle x_i^2 \rangle = \frac{1}{3}\langle r^2 \rangle = kTt/3\pi\eta R$.

A gas is called a *Knudsen gas* if $\ell \gg$ the dimensions of the gas, something that can easily occur at low pressures. The equilibrium condition for a vessel which has a hole with surface A in it for which holds that $\ell \gg \sqrt{A/\pi}$ is: $n_1\sqrt{T_1} = n_2\sqrt{T_2}$. Together with the general gas law follows: $p_1/\sqrt{T_1} = p_2/\sqrt{T_2}$.

If two plates move along each other at a distance d with velocity w_x the *viscosity* η is given by: $F_x = \eta\frac{Aw_x}{d}$. The velocity profile between the plates is in that case given by $w(z) = zw_x/d$. It can be derived that $\eta = \frac{1}{3}\varrho\ell\langle v \rangle$ where v is the *thermal velocity*.

The heat conductance in a non-moving gas is described by: $\frac{dQ}{dt} = \kappa A\left(\frac{T_2 - T_1}{d}\right)$, which results in a temperature profile $T(z) = T_1 + z(T_2 - T_1)/d$. It can be derived that $\kappa = \frac{1}{3}C_{mV}n\ell\langle v \rangle/N_\mathrm{A}$. Also holds: $\kappa = C_V\eta$. A better expression for κ can be obtained with the *Eucken correction*: $\kappa = (1 + 9R/4c_{mV})C_V \cdot \eta$ with an error <5%.

7.6 Interaction between molecules

For dipole interaction between molecules can be derived that $U \sim -1/r^6$. If the distance between two molecules approaches the molecular diameter D a repulsing force between the electron clouds appears. This force can be described by $U_\mathrm{rep} \sim \exp(-\gamma r)$ or $V_\mathrm{rep} = +C_s/r^s$ with $12 \leq s \leq 20$. This results in the *Lennard-Jones* potential for intermolecular forces:

$$U_\mathrm{LJ} = 4\epsilon\left[\left(\frac{D}{r}\right)^{12} - \left(\frac{D}{r}\right)^{6}\right]$$

with a minimum ϵ at $r = r_\mathrm{m}$. The following holds: $D \approx 0,89r_\mathrm{m}$. For the Van der Waals coefficients a and b and the critical quantities holds: $a = 5,275N_\mathrm{A}^2D^3\epsilon$, $b = 1,3N_\mathrm{A}D^3$, $kT_\mathrm{kr} = 1,2\epsilon$ and $V_\mathrm{m,kr} = 3,9N_\mathrm{A}D^3$.

A more simple model for intermolecular forces assumes a potential $U(r) = \infty$ for $r < D$, $U(r) = U_\mathrm{LJ}$ for $D \leq r \leq 3D$ and $U(r) = 0$ for $r \geq 3D$. This gives for the potential energy of one molecule: $E_\mathrm{pot} = \int\limits_D^{3D} U(r)F(r)dr$.

with $F(r)$ the spatial distribution function in spherical coordinates, which is for a homogeneous distribution given by: $F(r)dr = 4n\pi r^2dr$.

Some useful mathematical relations are:

$$\int\limits_0^\infty x^n e^{-x}dx = n!\ \ ,\ \ \int\limits_0^\infty x^{2n}e^{-x^2}dx = \frac{(2n)!\sqrt{\pi}}{n!2^{2n+1}}\ \ ,\ \ \int\limits_0^\infty x^{2n+1}e^{-x^2}dx = \tfrac{1}{2}n!$$

Chapter 8

Thermodynamics

8.1 Mathematical introduction

If there exists a relation $f(x,y,z)=0$ between 3 variables, one can write: $x=x(y,z)$, $y=y(x,z)$ and $z=z(x,y)$. The *total differential* dz of z is than given by:

$$dz=\left(\frac{\partial z}{\partial x}\right)_y dx+\left(\frac{\partial z}{\partial y}\right)_x dy$$

By writing this also for dx and dy it can be obtained that

$$\left(\frac{\partial x}{\partial y}\right)_z\cdot\left(\frac{\partial y}{\partial z}\right)_x\cdot\left(\frac{\partial z}{\partial x}\right)_y=-1$$

Because dz is a total differential holds $\oint dz=0$.

A homogeneous function of degree m obeys: $\varepsilon^m F(x,y,z)=F(\varepsilon x,\varepsilon y,\varepsilon z)$. For such a function Euler's theorem applies:

$$mF(x,y,z)=x\frac{\partial F}{\partial x}+y\frac{\partial F}{\partial y}+z\frac{\partial F}{\partial z}$$

8.2 Definitions

- The isochoric pressure coefficient: $\beta_V=\dfrac{1}{p}\left(\dfrac{\partial p}{\partial T}\right)_V$
- The isothermal compressibility: $\kappa_T=-\dfrac{1}{V}\left(\dfrac{\partial V}{\partial p}\right)_T$
- The isobaric volume coefficient: $\gamma_p=\dfrac{1}{V}\left(\dfrac{\partial V}{\partial T}\right)_p$
- The adiabatic compressibility: $\kappa_S=-\dfrac{1}{V}\left(\dfrac{\partial V}{\partial p}\right)_S$

For an ideal gas follows: $\gamma_p=1/T$, $\kappa_T=1/p$ and $\beta_V=-1/V$.

8.3 Thermal heat capacity

- The specific heat at constant X is: $C_X=T\left(\dfrac{\partial S}{\partial T}\right)_X$
- The specific heat at constant pressure: $C_p=\left(\dfrac{\partial H}{\partial T}\right)_p$
- The specific heat at constant volume: $C_V=\left(\dfrac{\partial U}{\partial T}\right)_V$

For an ideal gas holds: $C_{mp} - C_{mV} = R$. Further, if the temperature is high enough to thermalize all internal rotational and vibrational degrees of freedom, holds: $C_V = \frac{1}{2}sR$. So $C_p = \frac{1}{2}(s+2)R$. For their ratio now follows $\gamma = (2+s)/s$. For a lower T one needs only to consider the thermalized degrees of freedom. For a Van der Waals gas holds: $C_{mV} = \frac{1}{2}sR + ap/RT^2$.

In general holds:

$$C_p - C_V = T\left(\frac{\partial p}{\partial T}\right)_V \cdot \left(\frac{\partial V}{\partial T}\right)_p = -T\left(\frac{\partial V}{\partial T}\right)_p^2 \left(\frac{\partial p}{\partial V}\right)_T \geq 0$$

Because $(\partial p/\partial V)_T$ is always < 0, the following is always true: $C_p \geq C_V$. If the coefficient of expansion is 0, $C_p = C_V$, and also at $T = 0$K.

8.4 The laws of thermodynamics

The zeroth law is that heat flows from higher to lower temperatures. The first law is the conservation of energy. For a closed system holds: $Q = \Delta U + W$, where Q is the total added heat, W the performed work and ΔU the difference in the internal energy. In differential form this becomes: $đQ = dU + đW$, where $đ$ means that the it is not a differential of a quantity of state. For a quasi-statical process holds: $đW = pdV$. So for a reversible process holds: $đQ = dU + pdV$.

For an open (flowing) system the first law is: $Q = \Delta H + W_{\rm i} + \Delta E_{\rm kin} + \Delta E_{\rm pot}$. One can extract a work $W_{\rm t}$ from the system or add a work $W_{\rm t} = -W_{\rm i}$ to the system.

The second law is: there exists an additive quantity S, the entropy, whose differential has the following property:

$$dS \geq \frac{đQ}{T}$$

If the only processes occurring are reversible holds: $dS = đQ_{\rm rev}/T$. So, the entropy difference after a reversible process is:

$$S_2 - S_1 = \int\limits_1^2 \frac{đQ_{\rm rev}}{T}$$

So, for a reversible cycle holds: $\displaystyle\oint \frac{đQ_{\rm rev}}{T} = 0$.

For an irreversible cycle holds: $\displaystyle\oint \frac{đQ_{\rm irr}}{T} < 0$.

The third law of thermodynamics is (Nernst):

$$\lim_{T\to 0}\left(\frac{\partial S}{\partial X}\right)_T = 0$$

From this can be concluded that the thermal heat capacity → ∞ if $T \to 0$, so absolute zero temperature can not be reached by cooling with a finite number of steps.

8.5 State functions and Maxwell relations

The quantities of state and their differentials are:

Internal energy:	U	$dU = TdS - pdV$
Enthalpy:	$H = U + pV$	$dH = TdS + Vdp$
Free energy:	$F = U - TS$	$dF = -SdT - pdV$
Gibbs free enthalpy:	$G = H - TS$	$dG = -SdT + Vdp$

From this one can derive Maxwell's relations:

$$\left(\frac{\partial T}{\partial V}\right)_S=-\left(\frac{\partial p}{\partial S}\right)_V~,~~\left(\frac{\partial T}{\partial p}\right)_S=\left(\frac{\partial V}{\partial S}\right)_p~,~~\left(\frac{\partial p}{\partial T}\right)_V=\left(\frac{\partial S}{\partial V}\right)_T~,~~\left(\frac{\partial V}{\partial T}\right)_p=-\left(\frac{\partial S}{\partial p}\right)_T$$

From the complete differential and the definitions of C_V and C_p can be derived that:

$$TdS=C_VdT+T\left(\frac{\partial p}{\partial T}\right)_V dV~~\text{and}~~TdS=C_pdT-T\left(\frac{\partial V}{\partial T}\right)_p dp$$

For an ideal gas also holds:

$$S_m=C_V\ln\left(\frac{T}{T_0}\right)+R\ln\left(\frac{V}{V_0}\right)+S_{m0}~~\text{and}~~S_m=C_p\ln\left(\frac{T}{T_0}\right)-R\ln\left(\frac{p}{p_0}\right)+S'_{m0}$$

Helmholtz' equations are:

$$\left(\frac{\partial U}{\partial V}\right)_T=T\left(\frac{\partial p}{\partial T}\right)_V-p~~,~~\left(\frac{\partial H}{\partial p}\right)_T=V-T\left(\frac{\partial V}{\partial T}\right)_p$$

When a surface is enlarged holds: $\bar{d}W_{\rm rev}=-\gamma dA$, with γ the surface tension. From this follows:

$$\gamma=\left(\frac{\partial U}{\partial A}\right)_S=\left(\frac{\partial F}{\partial A}\right)_T$$

8.6 Processes

The *efficiency* η of a process is given by: $\eta=\dfrac{\text{Work done}}{\text{Heat added}}$

The *Cold factor* ξ of a cooling down process is given by: $\xi=\dfrac{\text{Cold delivered}}{\text{Work added}}$

Reversible adiabatic processes

For adiabatic processes holds: $W=U_1-U_2$. For reversible adiabatic processes holds Poisson's equation: with $\gamma=C_p/C_V$ one gets that pV^γ =constant. Also holds: $TV^{\gamma-1}$ =constant and $T^\gamma p^{1-\gamma}$ =constant. Adiabatics are more stylish in a p-V diagram than isothermics because $\gamma>1$.

Isobaric processes

Here holds: $H_2-H_1=\int_1^2 C_pdT$. For a reversible isobaric process holds: $H_2-H_1=Q_{\rm rev}$.

The throttle process

This is also called the *Joule-Kelvin* effect, and is an adiabatic expansion of a gas through a porous material or a small opening. Here is H a conserved quantity, and $dS>0$. In general this is acompanied with a change in temperature. The quantity which is important here is the *throttle coefficient*:

$$\alpha_H=\left(\frac{\partial T}{\partial p}\right)_H=\frac{1}{C_p}\left[T\left(\frac{\partial V}{\partial T}\right)_p-V\right]$$

The *inversion temperature* is the temperature where an adiabatically expanding gas keeps the same temperature If $T>T_{\rm i}$ the gas heats up, if $T<T_{\rm i}$ the gas cools down. $T_{\rm i}=2T_{\rm B}$, with for $T_{\rm B}$: $[\partial(pV)/\partial p]_T=0$. The throttle process is e.g. applied in refridgerators.

The Carnotprocess

The system undergoes a reversible cycle with 2 isothemics and 2 adiabatics:

1. Isothermic expansion at T_1. The system absorbs a heat Q_1 from the reservoir.
2. Adiabatic expansion with a temperature drop to T_2.

3. Isothermic compression at T_2, removing Q_2 from the system.
4. Adiabatic compression to T_1.

The efficiency for Carnot's process is:

$$\eta = 1 - \frac{|Q_2|}{|Q_1|} = 1 - \frac{T_2}{T_1} := \eta_{\rm C}$$

The *Carnot efficiency* $\eta_{\rm C}$ is the maximal efficiency at which a heat machine can operate. If the process is applied in reverse order and the system performs a work $-W$ the cold factor is given by:

$$\xi = \frac{|Q_2|}{W} = \frac{|Q_2|}{|Q_1| - |Q_2|} = \frac{T_2}{T_1 - T_2}$$

The Stirling process

Stirling's cycle exists of 2 isothermics and 2 isochorics. The efficiency in the ideal case is the same as for Carnot's cycle.

8.7 Maximal work

Consider a system that transits from state 1 to state 2, with the temperature and pressure of the surroundings given by T_0 and p_0. The maximum work which can be obtained from this change is, when all processes are reversible:

1. Closed system: $W_{\rm max} = (U_1 - U_2) - T_0(S_1 - S_2) + p_0(V_1 - V_2)$.
2. Open system: $W_{\rm max} = (H_1 - H_2) - T_0(S_1 - S_2) - \Delta E_{\rm kin} - \Delta E_{\rm pot}$.

The minimal work needed to reach a certain state is: $W_{\rm min} = -W_{\rm max}$.

8.8 Phase transitions

Phase transitions are isothermic and isobaric, so $dG = 0$. When the phases are noted with α, β and γ holds: $G_m^\alpha = G_m^\beta$ and

$$\Delta S_m = S_m^\alpha - S_m^\beta = \frac{r_{\beta\alpha}}{T_0}$$

where $r_{\beta\alpha}$ is the transition heat of phase β to phase α and T_0 is the transition temperature. The following holds: $r_{\beta\alpha} = r_{\alpha\beta}$ and $r_{\beta\alpha} = r_{\gamma\alpha} - r_{\gamma\beta}$. Further

$$S_m = \left(\frac{\partial G_m}{\partial T}\right)_p$$

so G has a twist in the transition point. In a two phase system holds Clapheyron's equation:

$$\frac{dp}{dT} = \frac{S_m^\alpha - S_m^\beta}{V_m^\alpha - V_m^\beta} = \frac{r_{\beta\alpha}}{(V_m^\alpha - V_m^\beta)T}$$

For an ideal gas one finds for the vapor line at some distance from the critical point:

$$p = p_0 {\rm e}^{-r_{\beta\alpha}/RT}$$

There exist also phase transitions with $r_{\beta\alpha} = 0$. For those there will occur only a discontinuity in the second derivates of G_m. These second-order transitions appear at *organization phenomena.*

A phase-change of the 3rd order, so with e.g. $[\partial^3 G_m/\partial T^3]_p$ non continuous arises e.g. when ferromagnetic iron changes to the paramagnetic state.

8.9 Thermodynamic potential

When the number of particles within a system changes this number becomes a third quantity of state. Because addition of matter usually happens at constant p and T, G is the relevant quantity. If a system exists of more components this becomes:

$$dG = -SdT + Vdp + \sum_i \mu_i dn_i$$

where $\mu = \left(\frac{\partial G}{\partial n_i}\right)_{p,T,n_j}$ is called the thermodynamic potential. This is a *partial quantity.* For V holds:

$$V = \sum_{i=1}^{c} n_i \left(\frac{\partial V}{\partial n_i}\right)_{n_j,p,T} := \sum_{i=1}^{c} n_i V_i$$

where V_i is the the partial volume of component i. The following holds:

$$\begin{aligned} V_m &= \sum_i x_i V_i \\ 0 &= \sum_i x_i dV_i \end{aligned}$$

where $x_i = n_i/n$ is the molar fraction of component i. The molar volume of a mixture of two components can be a concave line in a V-x_2 diagram: the mixing contracts the volume.

The thermodynamic potentials are not independent in a multiple-phase system. It can be derived that $\sum\limits_i n_i d\mu_i = -SdT + Vdp$, this gives at constant p and T: $\sum\limits_i x_i d\mu_i = 0$ (Gibbs-Duhmen).

Each component has as much μ's as there are phases. The number of free parameters in a system with c components and p different phases is given by $f = c + 2 - p$.

8.10 Ideal mixtures

For a mixture of n components holds (the index ^{0} is the value for the pure component):

$$U_{\rm mixture} = \sum_i n_i U_i^0 \quad , \quad H_{\rm mixture} = \sum_i n_i H_i^0 \quad , \quad S_{\rm mixture} = n \sum_i x_i S_i^0 + \Delta S_{\rm mix}$$

where for ideal gases holds: $\Delta S_{\rm mix} = -nR \sum\limits_i x_i \ln(x_i)$.

For the thermodynamic potentials holds: $\mu_i = \mu_i^0 + RT\ln(x_i) < \mu_i^0$. A mixture of two liquids is rarely ideal: this is usually only the case for chemical related components or isotopes. In spite of this holds Raoult's law for the vapor pressure holds for many binary mixtures: $p_i = x_i p_i^0 = y_i p$. Here is x_i the fraction of the ith component in liquid phase and y_i the fraction of the ith component in gas phase.

A solution of one component in another gives rise to an increase in the boiling point $\Delta T_{\rm k}$ and a decrease of the freezing point. $\Delta T_{\rm s}$. For $x_2 \ll 1$ holds:

$$\Delta T_{\rm k} = \frac{RT_{\rm k}^2}{r_{\beta\alpha}} x_2 \quad , \quad \Delta T_{\rm s} = -\frac{RT_{\rm s}^2}{r_{\gamma\beta}} x_2$$

with $r_{\beta\alpha}$ the evaporation heat and $r_{\gamma\beta} < 0$ the melting heat. For the *osmotic pressure* Π of a solution holds: $\Pi V_{ml}^0 = x_2 RT$.

8.11 Conditions for equilibrium

When a system evolves towards equilibrium the only changes that are possible are those for which holds: $(dS)_{U,V} \geq 0$ or $(dU)_{S,V} \leq 0$ or $(dH)_{S,p} \leq 0$ or $(dF)_{T,V} \leq 0$ or $(dG)_{T,p} \leq 0$. In equilibrium holds for each component: $\mu_i^\alpha = \mu_i^\beta = \mu_i^\gamma$.

8.12 Statistical basis for thermodynamics

The number of possibilities P to distribute N particles on n possible energy levels, each with a g-fold degeneracy is called the thermodynamic probability and is given by:

$$P = N!\prod_i \frac{g_i^{n_i}}{n_i!}$$

The most probable distribution, the one with the maximum value for P, is the *equilibrium state*. When Stirling's equation, $\ln(n!) \approx n\ln(n) - n$ is used, one finds for a discrete system the Maxwell-Boltzmann distribution. The occupation numbers in equilibrium are then given by:

$$n_i = \frac{N}{Z} g_i \exp\left(-\frac{W_i}{kT}\right)$$

The *state sum* Z is a norming constant, given by: $Z = \sum\limits_i g_i \exp(-W_i/kT)$. Fort an ideal gas holds:

$$Z = \frac{V(2\pi mkT)^{3/2}}{h^3}$$

The entropy can than be defined as: $\boxed{S = k\ln(P)}$. For a system in thermodynamic equilibrium this becomes:

$$S = \frac{U}{T} + kN\ln\left(\frac{Z}{N}\right) \approx \frac{U}{T} + k\ln\left(\frac{Z^N}{N!}\right)$$

For an ideal gas, with $U = \frac{3}{2}kT$ then holds: $S = \frac{5}{2}kN + kN\ln\left(\frac{V(2\pi mkT)^{3/2}}{Nh^3}\right)$

8.13 Application on other systems

Thermodynamics can be applied on other systems than gases and liquids. To do this the term $\bar{d}W = pdV$ has to be replaced with the correct work term, like $\bar{d}W_{\rm rev} = -Fdl$ for the stretching of a wire, $\bar{d}W_{\rm rev} = -\gamma dA$ for the expansion of a soap bubble or $\bar{d}W_{\rm rev} = -BdM$ for a magnetic system.

Chapter 9

Transport phenomena

9.1 Mathematical introduction

An important relation is: if X is a quantity of a volume element which travels from position $\vec{r}$ to $\vec{r}+d\vec{r}$ in a time dt, the total differential dX is then given by:

$$dX=\frac{\partial X}{\partial x}dx+\frac{\partial X}{\partial y}dy+\frac{\partial X}{\partial z}dz+\frac{\partial X}{\partial t}dt \;\Rightarrow\; \frac{dX}{dt}=\frac{\partial X}{\partial x}v_x+\frac{\partial X}{\partial y}v_y+\frac{\partial X}{\partial z}v_z+\frac{\partial X}{\partial t}$$

This results in general to: $\boxed{\dfrac{dX}{dt}=\dfrac{\partial X}{\partial t}+(\vec{v}\cdot\nabla)X}$.

From this follows that also holds: $\boxed{\dfrac{d}{dt}\iiint Xd^3V=\dfrac{\partial}{\partial t}\iiint Xd^3V+\oiint X(\vec{v}\cdot\vec{n})d^2A}$

when the volume V is surrounded by surface A. Some properties of the ∇ operator are:

$$\begin{array}{lll}
\mathrm{div}(\phi\vec{v})=\phi\mathrm{div}\vec{v}+\mathrm{grad}\phi\cdot\vec{v} & \mathrm{rot}(\phi\vec{v})=\phi\mathrm{rot}\vec{v}+(\mathrm{grad}\phi)\times\vec{v} & \mathrm{rot\ grad}\phi=\vec{0}\\
\mathrm{div}(\vec{u}\times\vec{v})=\vec{v}\cdot(\mathrm{rot}\vec{u})-\vec{u}\cdot(\mathrm{rot}\vec{v}) & \mathrm{rot\ rot}\vec{v}=\mathrm{grad\ div}\vec{v}-\nabla^2\vec{v} & \mathrm{div\ rot}\vec{v}=0\\
\mathrm{div\ grad}\phi=\nabla^2\phi & \nabla^2\vec{v}\equiv(\nabla^2v_1,\nabla^2v_2,\nabla^2v_3) &
\end{array}$$

Here, $\vec{v}$ is an arbitrary vector field and ϕ an arbitrary scalar field. Some important integral theorems are:

Gauss: $\oiint(\vec{v}\cdot\vec{n})d^2A=\iiint(\mathrm{div}\vec{v}\ )d^3V$

Stokes for a scalar field: $\oint(\phi\cdot\vec{e}_{\rm t})ds=\iint(\vec{n}\times\mathrm{grad}\phi)d^2A$

Stokes for a vector field: $\oint(\vec{v}\cdot\vec{e}_{\rm t})ds=\iint(\mathrm{rot}\vec{v}\cdot\vec{n})d^2A$

This results in: $\oiint(\mathrm{rot}\vec{v}\cdot\vec{n})d^2A=0$

Ostrogradsky: $\oiint(\vec{n}\times\vec{v}\ )d^2A=\iiint(\mathrm{rot}\vec{v}\ )d^3A$

$\oiint(\phi\vec{n})d^2A=\iiint(\mathrm{grad}\phi)d^3V$

Here, the orientable surface $\iint d^2A$ is limited by the Jordan curve $\oint ds$.

9.2 Conservation laws

On a volume work two kinds of forces:

1. The force $\vec{f}_0$ on each volume element. For gravity holds: $\vec{f}_0=\varrho\vec{g}$.
2. Surface forces working only on the margins: $\vec{t}$. For these holds: $\vec{t}=\vec{n}\ \mathsf{T}$, where T is the *pressure tensor*.

T can be split in a part $p\mathsf{I}$ representing the normal tensions and a part T' representing the shear stresses: $\mathsf{T} = \mathsf{T}' + p\mathsf{I}$, where I is the unit tensor. When viscous aspects can be ignored holds: div$\mathsf{T}$= $-$grad$p$.

When the flow velocity is $\vec{v}$ at position $\vec{r}$ holds on position $\vec{r} + d\vec{r}$:

$$\vec{v}(d\vec{r}) = \underbrace{\vec{v}(\vec{r})}_{\text{translation}} + \underbrace{d\vec{r}\cdot(\text{grad}\vec{v})}_{\text{rotation, deformation, dilatation}}$$

The quantity L:=grad$\vec{v}$ can be spilt in a symmetric part D and an antisymmetric part W. $\mathsf{L} = \mathsf{D} + \mathsf{W}$ with

$$D_{ij} := \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) \ , \ \ W_{ij} := \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}\right)$$

When the rotation or *vorticity* $\vec{\omega} = \text{rot}\vec{v}$ is introduced holds: $W_{ij} = \frac{1}{2}\varepsilon_{ijk}\omega_k$. $\vec{\omega}$ represents the local rotation velocity: $\vec{dr} \cdot \mathsf{W} = \frac{1}{2}\omega \times \vec{dr}$.

For a *Newtonian liquid* holds: $\mathsf{T}' = 2\eta\mathsf{D}$. Here, η is the dynamical viscosity. These is related with the shear stress τ by:

$$\tau_{ij} = \eta\frac{\partial v_i}{\partial x_j}$$

For compressible media can be stated: $\mathsf{T}' = (\eta'\text{div}\vec{v})\mathsf{I} + 2\eta\mathsf{D}$. Equilization of the thermodynamical and the mechanical pressure follows: $3\eta' + 2\eta = 0$. If the viscosity is constant holds: $\text{div}(2\mathsf{D}) = \nabla^2\vec{v} + \text{grad div}\vec{v}$.

The conservation laws for mass, momentum and energy for continuous media can be written in both integral and differential form. They are:

Integral notation:

1. Conservation of mass: $\displaystyle\frac{\partial}{\partial t}\iiint \varrho d^3V + \oiint \varrho(\vec{v}\cdot\vec{n})d^2A = 0$
2. Conservation of momentum: $\displaystyle\frac{\partial}{\partial t}\iiint \varrho\vec{v}d^3V + \oiint \varrho\vec{v}(\vec{v}\cdot\vec{n})d^2A = \iiint f_0 d^3V + \oiint \vec{n}\cdot T d^2A$
3. Conservation of energy: $\displaystyle\frac{\partial}{\partial t}\iiint (\tfrac{1}{2}v^2 + e)\varrho d^3V + \oiint (\tfrac{1}{2}v^2 + e)\varrho(\vec{v}\cdot\vec{n})d^2A =$

$$-\oiint (\vec{q}\cdot\vec{n})d^2A + \iiint(\vec{v}\cdot\vec{f_0})d^3V + \oiint (\vec{v}\cdot\vec{n}\ \mathsf{T})d^2A$$

Differential notation:

1. Conservation of mass: $\displaystyle\frac{\partial\varrho}{\partial t} + \text{div}\cdot(\varrho\vec{v}) = 0$
2. Conservation of momentum: $\displaystyle\varrho\frac{\partial\vec{v}}{\partial t} + (\varrho\vec{v}\cdot\nabla)\vec{v} = \vec{f_0} + \text{div}\mathsf{T} = \vec{f_0} - \text{grad}p + \text{div}\mathsf{T}'$
3. Conservation of energy: $\displaystyle\varrho T\frac{ds}{dt} = \varrho\frac{de}{dt} - \frac{p}{\varrho}\frac{d\varrho}{dt} = -\text{div}\vec{q} + \mathsf{T}' : \mathsf{D}$

Here, e is the internal energy per unit of mass E/m and s is the entropy per unit of mass S/m. $\vec{q} = -\kappa\vec{\nabla}T$ is the heat flow. Further holds:

$$p = -\frac{\partial E}{\partial V} = -\frac{\partial e}{\partial 1/\varrho} \ , \ \ T = \frac{\partial E}{\partial S} = \frac{\partial e}{\partial s}$$

so

$$C_V = \left(\frac{\partial e}{\partial T}\right)_V \ \ \text{and} \ \ C_p = \left(\frac{\partial h}{\partial T}\right)_p$$

with $h = H/m$ the enthalpy per unit of mass.

From this one can derive the *Navier-Stokes* equations for an incompressible, viscous and heat-conducting medium:

$$\begin{aligned}\mathrm{div}\vec{v} &= 0\\ \varrho\frac{\partial\vec{v}}{\partial t} + \varrho(\vec{v}\cdot\nabla)\vec{v} &= \varrho\vec{g} - \mathrm{grad}p + \eta\nabla^2\vec{v}\\ \varrho C\frac{\partial T}{\partial t} + \varrho C(\vec{v}\cdot\nabla)T &= \kappa\nabla^2 T + 2\eta\mathsf{D}:\mathsf{D}\end{aligned}$$

with C the thermal heat capacity. The force $\vec{F}$ on an object within a flow, when viscous effects are limited to the boundary layer, can be obtained using the momentum law. If a surface A surrounds the object outside the boundary layer holds:

$$\vec{F} = -\oiint[p\vec{n} + \varrho\vec{v}(\vec{v}\cdot\vec{n})]d^2A$$

9.3 Bernoulli's equations

Starting with the momentum equation one can find for a non-viscous medium for stationary flows, with

$$(\vec{v}\cdot\mathrm{grad})\vec{v} = \tfrac{1}{2}\mathrm{grad}(v^2) + (\mathrm{rot}\vec{v})\times\vec{v}$$

and the potential equation $\vec{g} = -\mathrm{grad}(gh)$ that:

$$\tfrac{1}{2}v^2 + gh + \int\frac{dp}{\varrho} = \text{constant along a streamline}$$

For compressible flows holds: $\frac{1}{2}v^2 + gh + p/\varrho$ =constant along a line of flow. If also holds $\mathrm{rot}\vec{v} = 0$ and the entropy is equal on each streamline holds $\frac{1}{2}v^2 + gh + \int dp/\varrho$ =constant everywhere. For incompressible flows this becomes: $\frac{1}{2}v^2 + gh + p/\varrho$ =constant everywhere. For ideal gases with constant C_p and C_V holds, with $\gamma = C_p/C_V$:

$$\tfrac{1}{2}v^2 + \frac{\gamma}{\gamma-1}\frac{p}{\varrho} = \tfrac{1}{2}v^2 + \frac{c^2}{\gamma-1} = \text{constant}$$

With a velocity potential defined by $\vec{v} = \mathrm{grad}\phi$ holds for instationary flows:

$$\frac{\partial\phi}{\partial t} + \tfrac{1}{2}v^2 + gh + \int\frac{dp}{\varrho} = \text{constant everywhere}$$

9.4 Caracterising of flows with dimensionless numbers

The advantage of dimensionless numbers is that they make model experiments possible: one has to make the dimensionless numbers which are important for the specific experiment equal for both model and the real situation. One can also deduce functional equalities without solving the differential equations. Some dimensionless numbers are given by:

Mach: $\mathrm{Ma} = \dfrac{v}{c}$

Strouhal: $\mathrm{Sr} = \dfrac{\omega L}{v}$

Fourier: $\mathrm{Fo} = \dfrac{a}{\omega L^2}$

Prandtl: $\mathrm{Pr} = \dfrac{\nu}{a}$

Eckert: $\mathrm{Ec} = \dfrac{v^2}{c\Delta T}$

Reynolds: $\mathrm{Re} = \dfrac{vL}{\nu}$

Froude: $\mathrm{Fr} = \dfrac{v^2}{gL}$

Péclet: $\mathrm{Pe} = \dfrac{vL}{a}$

Nusselt: $\mathrm{Nu} = \dfrac{L\alpha}{\kappa}$

Here, $\nu = \eta/\varrho$ is the *kinematic viscosity*, c is the speed of sound and L is a characteristic length of the system. α follows from the equation for heat transport $\kappa\partial_y T = \alpha\Delta T$ and $a = \kappa/\varrho c$ is the thermal diffusion coefficient.

These numbers can be interpreted as follows:

- Re: (stationary inertial forces)/(viscous forces)
- Sr: (instationary inertial forces)/(stationary inertial forces)
- Fr: (stationary inertial forces)/(gravity)
- Fo: (heat conductance)/(instationary change in enthalpy)
- Pe: (convective heat transport)/(heat conductance)
- Ec: (viscous dissipation)/(convective heat transport)
- Pr and Nu are related to specific materials.

Now, the dimensionless Navier-Stokes equation becomes, with $x' = x/L$, $\vec{v}\,' = \vec{v}/V$, $\text{grad}' = L\text{grad}$, $\nabla'^2 = L^2\nabla^2$ and $t' = t\omega$:

$$\text{Sr}\frac{\partial\vec{v}\,'}{\partial t'} + (\vec{v}\,'\cdot\nabla')\vec{v}\,' = -\text{grad}'p + \frac{\vec{g}}{\text{Fr}} + \frac{\nabla'^2\vec{v}\,'}{\text{Re}}$$

9.5 Tube flows

For tube flows holds: they are laminar if Re< 2300 with as dimension of length the diameter of the tube, and turbulent if Re is larger. For an incompressible laminar flow through a straight, circular tube holds for the velocity profile:

$$v(r) = -\frac{1}{4\eta}\frac{dp}{dx}(R^2 - r^2)$$

For the volume flow holds: $\Phi_V = \int\limits_0^R v(r)2\pi r dr = -\frac{\pi}{8\eta}\frac{dp}{dx}R^4$

The *entrance length* L_e is given by:

1. $500 < \text{Re}_D < 2300$: $L_\text{e}/2R = 0{,}056\text{Re}_D$
2. $\text{Re} > 2300$: $L_\text{e}/2R \approx 50$

For gas transport at low pressures (Knudsen-gas) holds: $\Phi_V = \frac{4R^3\alpha\sqrt{\pi}}{3}\frac{dp}{dx}$

For flows at a small Re holds: $\nabla p = \eta\nabla^2\vec{v}$ and $\text{div}\vec{v} = 0$. For the total force on a sphere with radius R in a flow then holds: $F = 6\pi\eta R v$. For large Re holds for the force on a surface A: $F = \frac{1}{2}C_W A\varrho v^2$.

9.6 Potential theory

The *circulation* Γ is defined as: $\Gamma = \oint(\vec{v}\cdot\vec{e}_\text{t})ds = \iint(\text{rot}\vec{v})\cdot\vec{n}d^2A = \iint(\vec{\omega}\cdot\vec{n})d^2A$

For non viscous media, if $p = p(\varrho)$ and all forces are conservative, Kelvin's theorem can be derived:

$$\frac{d\Gamma}{dt} = 0$$

For rotationless flows a velocity potential $\vec{v} = \text{grad}\phi$ can be introduced. In the incompressible case follows from conservation of mass $\nabla^2\phi = 0$. For a 2-dimensional flow a flow function $\psi(x,y)$ can be defined: with Φ_{AB} the amount of liquid flowing through a curve s between the points A and B:

$$\Phi_{AB} = \int\limits_A^B (\vec{v}\cdot\vec{n})ds = \int\limits_A^B (v_x dy - v_y dx)$$

and the definitions $v_x = \partial\psi/\partial y$, $v_y = -\partial\psi/\partial x$ holds: $\Phi_{AB} = \psi(B) - \psi(A)$. In general holds:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = -\omega_z$$

In polar coordinates holds:

$$v_r = \frac{1}{r}\frac{\partial\psi}{\partial\theta} = \frac{\partial\phi}{\partial r} \quad , \quad v_\theta = -\frac{\partial\psi}{\partial r} = \frac{1}{r}\frac{\partial\phi}{\partial\theta}$$

For source flows with power Q in $(x,y) = (0,0)$ holds: $\phi = \dfrac{Q}{2\pi}\ln(r)$ so that $v_r = Q/2\pi r$, $v_\theta = 0$.

For a dipole of strength Q in $x = a$ and strength $-Q$ in $x = -a$ follows from superposition: $\phi = -Qax/2\pi r^2$ where Qa is the dipole strength. For a vortex holds: $\phi = \Gamma\theta/2\pi$.

If an object is surrounded with an uniform main flow with $\vec{v} = v\vec{e}_x$ and such a large Re that viscous effects are limited to the boundary layer holds: $F_x = 0$ and $F_y = -\varrho\Gamma v$. The statement that $F_x = 0$ is d'Alembert's paradox and originates from the neglection of viscous effects. The lift F_y is also created by η because $\Gamma \neq 0$ due to viscous effects. So also rotating bodies create a force perpendicular to their direction of motion: the *Magnus effect*.

9.7 Boundary layers

9.7.1 Flow boundary layers

If for the thickness of the boundary layer holds: $\delta \ll L$ holds: $\delta \approx L/\sqrt{\text{Re}}$. With v_∞ the velocity of the main flow follows for the velocity $v_y \perp$ the surface: $v_y L \approx \delta v_\infty$. Blasius' equation for the boundary layer is, with $v_y/v_\infty = f(y/\delta)$: $2f''' + ff'' = 0$ with boundary conditions $f(0) = f'(0) = 0$, $f'(\infty) = 1$. From this follows: $C_W = 0{,}664\ \text{Re}_x^{-1/2}$.

The momentum theorem of Von Karman for the boundary layer is: $\dfrac{d}{dx}(\vartheta v^2) + \delta^* v\dfrac{dv}{dx} = \dfrac{\tau_0}{\varrho}$

where the displacement thickness $\delta^* v$ and the momentum thickness ϑv^2 are given by:

$$\vartheta v^2 = \int\limits_0^\infty (v - v_x)v_x dy \quad , \quad \delta^* v = \int\limits_0^\infty (v - v_x)dy \ \text{ and } \ \tau_0 = -\eta \left.\frac{\partial v_x}{\partial y}\right|_{y=0}$$

The boundary layer is released from the surface if $\left(\dfrac{\partial v_x}{\partial y}\right)_{y=0} = 0$. This is equivalent with $\dfrac{dp}{dx} = \dfrac{12\eta v_\infty}{\delta^2}$.

9.7.2 Temperature boundary layers

If the thickness of the temperature boundary layer $\delta_T \ll L$ holds:

1. If $\text{Pr} \leq 1$: $\delta/\delta_T \approx \sqrt{\text{Pr}}$.
2. If $\text{Pr} \gg 1$: $\delta/\delta_T \approx \sqrt[3]{\text{Pr}}$.

9.8 Heat conductance

For instationairy heat conductance in one dimension without flow holds:

$$\frac{\partial T}{\partial t}=\frac{\kappa}{\varrho c}\frac{\partial^2 T}{\partial x^2}+\Phi$$

where Φ is a source term. If $\Phi=0$ the solutions for harmonic oscillations at $x=0$ are:

$$\frac{T-T_\infty}{T_{\rm max}-T_\infty}=\exp\left(-\frac{x}{D}\right)\cos\left(\omega t-\frac{x}{D}\right)$$

with $D=\sqrt{2\kappa/\omega\varrho c}$. At $x=\pi D$ the temperature variation is in anti-phase with the surface. The one-dimensional solution at $\Phi=0$ is

$$T(x,t)=\frac{1}{2\sqrt{\pi a t}}\exp\left(-\frac{x^2}{4at}\right)$$

This is mathematical equivalent with the diffusion problem:

$$\frac{\partial n}{\partial t}=D\nabla^2 n+P-A$$

where P is the production of and A the discharge of particles. The flow density $J=-D\nabla n$.

9.9 Turbulence

The time scale of turbulent velocity variations $\tau_{\rm t}$ is in the order of: $\tau_{\rm t}=\tau\sqrt{\rm Re}/{\rm Ma}^2$ with τ the molecular time scale. For the velocity of the particles holds: $v(t)=\langle v\rangle+v'(t)$ with $\langle v'(t)\rangle=0$. The Navier-Stokes equation now becomes:

$$\frac{\partial\langle\vec{v}\,\rangle}{\partial t}+(\langle\vec{v}\,\rangle\cdot\nabla)\langle\vec{v}\,\rangle=-\frac{\nabla\langle p\rangle}{\varrho}+\nu\nabla^2\langle\vec{v}\,\rangle+\frac{{\rm div}\mathsf{S}_R}{\varrho}$$

where $\mathsf{S}_{Rij}=-\varrho\langle v_i v_j\rangle$ is the turbulent stress tensor. Boussinesq's assumption is: $\tau_{ij}=-\varrho\left\langle v_i' v_j'\right\rangle$. It is stated that, analogous to Newtonian media: $\mathsf{S}_R=2\varrho\nu_t\langle\mathsf{D}\rangle$. Near a boundary holds: $\nu_t=0$, far away of a boundary holds: $\nu_t\approx\nu{\rm Re}$.

9.10 Self organization

For a (semi) two-dimensional flow holds: $\dfrac{d\omega}{dt}=\dfrac{\partial\omega}{\partial t}+J(\omega,\psi)=\nu\nabla^2\omega$

With $J(\omega,\psi)$ the Jacobian. So if $\nu=0$ is ω is conserved. Further, the kinetic energy/mA and the enstrofy V are conserved: with $\vec{v}=\nabla\times(\vec{k}\psi)$

$$E\sim(\nabla\psi)^2\sim\int\limits_0^\infty\mathcal{E}(k,t)dk=\text{constant}\quad,\quad V\sim(\nabla^2\psi)^2\sim\int\limits_0^\infty k^2\mathcal{E}(k,t)dk=\text{constant}$$

From this follows that in a two-dimensional flow the energy flux goes towards large values of k: larger structures become larger at the expanse of smaller ones. In three-dimensional flows the situation is just the opposite.

Chapter 10

Quantum physics

10.1 Introduction in quantum physics

10.1.1 Black body radiation

Planck's law for the energy distribution for the radiation from a black body is:

$$w(f)=\frac{8\pi hf^3}{c^3}\frac{1}{\mathrm{e}^{hf/kT}-1}\quad,\quad w(\lambda)=\frac{8\pi hc}{\lambda^5}\frac{1}{\mathrm{e}^{hc/\lambda kT}-1}$$

Stefan-Boltzmann's law for the total power density can be derived from this: $P=A\sigma T^4$. Wien's law for the maximum can also be derived from this: $T\lambda_{\rm max}=k_{\rm W}$.

10.1.2 The Compton effect

For the wavelength of scattered light, if light is considered to exist of particles, can can be derived:

$$\lambda'=\lambda+\frac{h}{mc}(1-\cos\theta)=\lambda+\lambda_{\rm C}(1-\cos\theta)$$

10.1.3 Electron diffraction

Diffraction of electrons at a crystal can be explained by assuming that particles have a wave character with wavelength $\lambda=h/p$. This wavelength is called the Broglie-wavelength.

10.2 Wave functions

The wave character of particles is described with a wavefunction ψ. This wavefunction can be described in normal or momentum space. Both definitions are each others Fourier transformed:

$$\Phi(k,t)=\frac{1}{\sqrt{h}}\int\Psi(x,t)\mathrm{e}^{-ikx}dx\quad\text{and}\quad\Psi(x,t)=\frac{1}{\sqrt{h}}\int\Phi(k,t)\mathrm{e}^{ikx}dk$$

These waves define a particle with group velocity $v_{\rm g}=p/m$ and energy $E=\hbar\omega$.

The wavefunction can be interpreted as a measure for the probability P to find a particle somewhere (Born): $dP=|\psi|^2d^3V$. The expectation value $\langle f\rangle$ of a quantity f of a system is given by:

$$\langle f(t)\rangle=\iiint\Psi^*f\Psi d^3V\quad,\quad\langle f_p(t)\rangle=\iiint\Phi^*f\Phi d^3V_p$$

This is also written as $\langle f(t)\rangle=\langle\Phi|f|\Phi\rangle$. The normalizing condition for wavefunctions follows from this: $\langle\Phi|\Phi\rangle=\langle\Psi|\Psi\rangle=1$.

10.3 Operators in quantum physics

In quantum mechanics, classical quantities are translated in operators. These operators are hermitian because their eigenvalues must be real:

$$\int\psi_1^*A\psi_2d^3V=\int\psi_2(A\psi_1)^*d^3V$$

When u_n is the eigenfunction of the eigenvalue equation $A\Psi = a\Psi$ for eigenvalue a_n, Ψ can be developed to a basis of eigenfunctions: $\Psi = \sum\limits_n c_n u_n$. If this basis is chosen orthonormal, then follows for the coefficients: $c_n = \langle u_n|\Psi\rangle$. If the system is in a state described by Ψ, the chance to find eigenvalue a_n when measuring A is given by $|c_n|^2$ in the discrete part of the spectrum and $|c_n|^2 da$ in the continuous part of the spectrum between a and $a + da$. The *matrix element* A_{ij} is given by: $A_{ij} = \langle u_i|A|u_j\rangle$. Because $(AB)_{ij} = \langle u_i|AB|u_j\rangle = \langle u_i|A\sum\limits_n |u_n\rangle\langle u_n|B|u_j\rangle$ holds: $\sum\limits_n |u_n\rangle\langle u_n| = 1$.

The time-dependence of an operator is given by (Heisenberg):

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{[A,H]}{i\hbar}$$

with $[A,B] \equiv AB - BA$ the *commutator* of A and B. For hermitian operators the commutator is always complex. If $[A,B] = 0$, the operators A and B have a common set eigenfunctions. By applying this to p_x and x follows (Ehrenfest):

$$m\frac{d^2}{dt^2}\langle x\rangle_t = -\left\langle \frac{dU(x)}{dx}\right\rangle$$

The first order approximation $\langle F(x)\rangle_t \approx F(\langle x\rangle)$, with $F = -dU/dx$ represents the classical equation.

10.4 The uncertaincy principle

If the uncertaincy ΔA in A is defined as: $(\Delta A)^2 = \left\langle \psi|A_{\rm op} - \langle A\rangle|^2\psi\right\rangle = \left\langle A^2\right\rangle - \langle A\rangle^2$ follows:

$$\Delta A \cdot \Delta B \geq \tfrac{1}{2}|\langle\psi|[A,B]|\psi\rangle|$$

From this follows: $\Delta E \cdot \Delta t \geq \frac{1}{2}\hbar$, and because $[x, p_x] = i\hbar$ holds: $\Delta p_x \cdot \Delta x \geq \frac{1}{2}\hbar$, and $\Delta L_x \cdot \Delta L_y \geq \frac{1}{2}\hbar L_z$.

10.5 The Schrödinger equation

The momentum operator is given by: $p_{\rm op} = -i\hbar\nabla$. The position operator is: $x_{\rm op} = i\hbar\nabla_p$. The energy operator is given by: $E_{\rm op} = i\hbar\partial/\partial t$. The Hamiltonian of a particle with mass m, potential energy U and total energy E is given by: $H = p^2/2m + U$. From $H\psi = E\psi$ then follows the *Schrödinger equation*:

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

The linear combination of the solutions of this equation form the general solution. In one dimension it is:

$$\psi(x,t) = \left(\sum + \int dE\right) c(E)u_E(x)\exp\left(-\frac{iEt}{\hbar}\right)$$

The current density J is given by: $J = \dfrac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*)$

The following conservation law holds: $\dfrac{\partial P(x,t)}{\partial t} = -\nabla J(x,t)$

10.6 Parity

The parity operator in one dimension is given by $\mathcal{P}\psi(x) = \psi(-x)$. If the wavefunction is split in even and odd functions, it is being developed to eigenfunctions of $\mathcal{P}$:

$$\psi(x) = \underbrace{\tfrac{1}{2}(\psi(x) + \psi(-x))}_{\text{even: }\psi^+} + \underbrace{\tfrac{1}{2}(\psi(x) - \psi(-x))}_{\text{odd: }\psi^-}$$

$[\mathcal{P}, H] = 0$. The functions $\psi^+ = \frac{1}{2}(1+\mathcal{P})\psi(x,t)$ and $\psi^- = \frac{1}{2}(1-\mathcal{P})\psi(x,t)$ both satisfy the Schrödinger equation. So parity is a conserved quantity.

10.7 The tunnel effect

The wavefunction of a particle in an ∞ high potential step from $x = 0$ to $x = a$ is given by $\psi(x) = a^{-1/2}\sin(kx)$. The energylevels are given by $E_n = n^2h^2/8a^2m$.

If the wavefunction with energy W meets a potential well of $W_0 > W$ the wavefunction will, unlike the classical case, be non-zero within the potential well. If 1, 2 and 3 are the areas before, within and after the potential well, holds:

$$\psi_1 = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx} \quad , \quad \psi_2 = C\mathrm{e}^{ik'x} + D\mathrm{e}^{-ik'x} \quad , \quad \psi_3 = A'\mathrm{e}^{ikx}$$

with $k'^2 = 2m(W - W_0)/\hbar^2$ and $k^2 = 2mW$. Using the boundary conditions requiring continuity: ψ =continuous and $\partial\psi/\partial x$ =continuous at $x = 0$ and $x = a$ gives B, C and D and A' expressed in A. The amplitude T of the transmitted wave is defined by $T = |A'|^2/|A|^2$. If $W > W_0$ and $2a = n\lambda' = 2\pi n/k'$ holds: $T = 1$.

10.8 The harmonic oscillator

For a harmonic oscillator holds: $U = \frac{1}{2}bx^2$ and $\omega_0^2 = b/m$. The Hamiltonian H is then given by:

$$H = \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2x^2 = \tfrac{1}{2}\hbar\omega + \omega A^\dagger A$$

with

$$A = \sqrt{\tfrac{1}{2}m\omega}x + \frac{ip}{\sqrt{2m\omega}} \quad \text{and} \quad A^\dagger = \sqrt{\tfrac{1}{2}m\omega}x - \frac{ip}{\sqrt{2m\omega}}$$

$A \neq A^\dagger$ is non hermitian. $[A, A^\dagger] = \hbar$ and $[A, H] = \hbar\omega A$. A is a raising *ladder operator*, $A^\dagger$ a lowering ladder operator. $HAu_E = (E - \hbar\omega)Au_E$. There is an eigenfunction u_0 for which holds: $Au_0 = 0$. The energy in this ground state is $\frac{1}{2}\hbar\omega$: the zero point energy. For the normalized eigenfunctions follows:

$$u_n = \frac{1}{\sqrt{n!}}\left(\frac{A^\dagger}{\sqrt{\hbar}}\right)^n u_0 \quad \text{with} \quad u_0 = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

with $E_n = (\frac{1}{2} + n)\hbar\omega$.

10.9 Angular momentum

For the angular momentum operators L holds: $[L_z, L^2] = 0$ and $[L, H] = 0$. However, cyclically holds: $[L_x, L_y] = i\hbar L_z$. Not all components of L can be known at the same time with arbitrary accuracy. For L_z holds:

$$L_z = -i\hbar\frac{\partial}{\partial\varphi} = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

The ladder operators $L_\pm$ are defined by: $L_\pm = L_x \pm iL_y$. Now holds: $L^2 = L_+L_- + L_z^2 - \hbar L_z$. Further,

$$L_\pm = \hbar\mathrm{e}^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\varphi}\right)$$

From $[L_+, L_z] = -\hbar L_+$ follows: $L_z(L_+Y_{lm}) = (m+1)\hbar(L_+Y_{lm})$.

From $[L_-, L_z] = \hbar L_-$ follows: $L_z(L_-Y_{lm}) = (m-1)\hbar(L_-Y_{lm})$.

From $[L^2, L_\pm] = 0$ follows: $L^2(L_\pm Y_{lm}) = l(l+1)\hbar^2(L_\pm Y_{lm})$.

Because L_x and L_y are hermitian (this implies $L_\pm^\dagger = L_\mp$) and $|L_\pm Y_{lm}|^2 > 0$ follows: $l(l+1) - m^2 - m \geq 0 \Rightarrow -l \leq m \leq l$. Further follows that l has to be integral or half-integral. Half-odd integral values give no unique solution ψ and are therefore dismissed.

10.10 Spin

For the spin operators are defined by their commutation relations: $[S_x, S_y] = i\hbar S_z$. Because the spin operators do not act in the physical space (x, y, z) the uniqueness of the wavefunction is not a criterium here: also half odd-integer values are allowed for the spin. Because $[L, S] = 0$ spin and angular momentum operators do not have a common set of eigenfunctions. The spin operators are given by $\vec{\vec{S}} = \frac{1}{2}\hbar\vec{\vec{\sigma}}$, with

$$\vec{\vec{\sigma}}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \ \vec{\vec{\sigma}}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \ , \ \vec{\vec{\sigma}}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The eigenstates of S_z are called *spinors*: $\chi = \alpha_+\chi_+ + \alpha_-\chi_-$, where $\chi_+ = (1, 0)$ represents the state with spin up ($S_z = \frac{1}{2}\hbar$) and $\chi_- = (0, 1)$ represents the state with spin down ($S_z = -\frac{1}{2}\hbar$). Then the probability to find spin up after a measurement is given by $|\alpha_+|^2$ and the chance to find spin down is given by $|\alpha_-|^2$. Of course holds $|\alpha_+|^2 + |\alpha_-|^2 = 1$.

The electron will have an intrinsic magnetic dipole moment $\vec{M}$ by virtue of its spin, given by $\vec{M} = -eg_S\vec{S}/2m$, with $g_S = 2(1 + \alpha/2\pi + \cdots)$ the gyromagnetic ratio. In the presence of an external magnetic field this gives a potential energy $U = -\vec{M} \cdot \vec{B}$. The Schrödinger equation then becomes because $\partial\chi/\partial x_i \equiv 0$:

$$i\hbar\frac{\partial\chi(t)}{\partial t} = \frac{eg\hbar}{4m}\vec{\sigma} \cdot \vec{B}\chi(t)$$

with $\vec{\sigma} = (\vec{\vec{\sigma}}_x, \vec{\vec{\sigma}}_y, \vec{\vec{\sigma}}_z)$. If $\vec{B} = B\vec{e}_z$ there are two eigenvalues for this problem: $\chi_\pm$ for $E = \pm eg\hbar B/4m = \pm\hbar\omega$. So the general solution is given by $\chi = (a\mathrm{e}^{-i\omega t}, b\mathrm{e}^{i\omega t})$. From this can be derived: $\langle S_x\rangle = \frac{1}{2}\hbar\cos(2\omega t)$ and $\langle S_y\rangle = \frac{1}{2}\hbar\sin(2\omega t)$. Thus the spin precesses about the z-axis with frequency 2ω. This causes the normal Zeeman splitting of spectral lines.

The potential operator for two particles with spin $\pm\frac{1}{2}\hbar$ is given by:

$$V(r) = V_1(r) + \frac{1}{\hbar^2}(\vec{S}_1 \cdot \vec{S}_2)V_2(r) = V_1(r) + \tfrac{1}{2}V_2(r)[S(S+1) - \tfrac{3}{2}]$$

This makes it possible for two states to exist: $S = 1$ (triplet) or $S = 0$ (Singlet).

10.11 The Dirac formalism

If the operators for p and E are substituted in the relativistic $E^2 = m_0^2c^4 + p^2c^2$ follows the *Klein-Gordon* equation:

$$\boxed{\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m_0^2c^2}{\hbar^2}\right)\psi(\vec{x}, t) = 0}$$

The operator $\Box - m_0^2c^2/\hbar^2$ can be separated:

$$\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m_0^2c^2}{\hbar^2} = \left\{\gamma_\lambda\frac{\partial}{\partial x_\lambda} - \frac{m_0^2c^2}{\hbar^2}\right\}\left\{\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{m_0^2c^2}{\hbar^2}\right\}$$

where the Dirac matrices γ are given by: $\gamma_\lambda\gamma_\mu + \gamma_\mu\gamma_\lambda = 2\delta_{\lambda\mu}$. From this it can be derived that the γ are hermitian 4×4 matrices given by:

$$\gamma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix} \ , \ \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

With this, the Dirac equation becomes:

$$\boxed{\left(\gamma_\lambda\frac{\partial}{\partial x_\lambda} + \frac{m_0^2c^2}{\hbar^2}\right)\psi(\vec{x}, t) = 0}$$

where $\psi(x) = (\psi_1(x), \psi_2(x), \psi_3(x), \psi_4(x))$ is a spinor.

10.12 Atom physics

10.12.1 Solutions

The solutions of the Schrödinger equation in spherical coordinates if the potential energy is a function of r alone can be written as: $\psi(r,\theta,\varphi)=R_{nl}(r)Y_{l,m_l}(\theta,\varphi)\chi_{m_s}$, with

$$Y_{lm}=\frac{C_{lm}}{\sqrt{2\pi}}P_l^m(\cos\theta)\mathrm{e}^{im\varphi}$$

For an atom or ion with one electron holds: $R_{lm}(\rho)=C_{lm}\mathrm{e}^{-\rho/2}\rho^l L_{n-l-1}^{2l+1}(\rho)$

with $\rho=2rZ/na_0$ with $a_0=\varepsilon_0 h^2/\pi m e^2 m_\mathrm{e}$. The L_i^j are the associated Laguere functions and the P_l^m are the associated Legendre polynomials:

$$P_l^{|m|}(x)=(1-x^2)^{m/2}\frac{d^{|m|}}{dx^{|m|}}\left[(x^2-1)^l\right] \quad , \quad L_n^m(x)=\frac{(-1)^m n!}{(n-m)!}\mathrm{e}^{-x}x^{-m}\frac{d^{n-m}}{dx^{n-m}}(\mathrm{e}^{-x}x^n)$$

The parity of these solutions is $(-1)^l$. The functions are $2\sum\limits_{l=0}^{n-1}(2l+1)=2n^2$-folded degenerated.

10.12.2 Eigenvalue equations

The eigenvalue equation for an atom or ion with with one electron are:

Equation	Eigenvalue	Range
$H_\mathrm{op}\psi=E\psi$	$E_n=\mu e^4Z^2/8\varepsilon_0^2h^2n^2$	$n\geq 1$
$L_{z\mathrm{op}}Y_{lm}=L_zY_{lm}$	$L_z=m_l\hbar$	$-l\leq m_l\leq l$
$L_\mathrm{op}^2Y_{lm}=L^2Y_{lm}$	$L^2=l(l+1)\hbar^2$	$l<n$
$S_{z\mathrm{op}}\chi=S_z\chi$	$S_z=m_s\hbar$	$m_s=\pm\frac{1}{2}$
$S_\mathrm{op}^2\chi=S^2\chi$	$S^2=s(s+1)\hbar^2$	$s=\frac{1}{2}$

10.12.3 Spin-orbit interaction

The total momentum is given by $\vec{J}=\vec{L}+\vec{M}$. The total magnetic dipole moment of an electron is then $\vec{M}=\vec{M}_L+\vec{M}_S=-(e/2m_\mathrm{e})(\vec{L}+g_S\vec{S})$ where $g_S=2,0024$ is the gyromagnetic ratio of the electron. Further holds: $J^2=L^2+S^2+2\vec{L}\cdot\vec{S}=L^2+S^2+2L_zS_z+L_+S_-+L_-S_+$. J has quantum numbers j with possible values $j=l\pm\frac{1}{2}$, with $2j+1$ possible z-components ($m_J\in\{-j,..,0,..,j\}$). If the interaction energy between S and L is small it can be stated that: $E=E_n+E_{SL}=E_n+a\vec{S}\cdot\vec{L}$. It can then be derived that:

$$a=\frac{|E_n|Z^2\alpha^2}{\hbar^2 nl(l+1)(l+\frac{1}{2})}$$

After a relativistic correction this becomes:

$$E=E_n+\frac{|E_n|Z^2\alpha^2}{n}\left(\frac{3}{4n}-\frac{1}{j+\frac{1}{2}}\right)$$

The *fine structure* in atomic spectra arises from this. With $g_S=2$ follows for the average magnetic moment: $\vec{M}_\mathrm{gem}=-(e/2m_\mathrm{e})g\hbar\vec{J}$, where g is the Landé-factor:

$$g=1+\frac{\vec{S}\cdot\vec{J}}{J^2}=1+\frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}$$

For atoms with more than one electron the following limiting situations occur:

1. $L-S$ coupling: for small atoms is the electrostatic interaction dominant and the state can be characterized by L,S,J,m_J. $J\in\{|L-S|,...,L+S-1,L+S\}$ and $m_J\in\{-J,...,J-1,J\}$. The spectroscopic notation for this interaction is: ${}^{2S+1}L_J$. $2S+1$ is the multiplicity of a multiplet.
2. $j-j$ coupling: for larger atoms is the electrostatic interaction smaller then the $L_i\cdot s_i$ interaction of an electron. The state is characterized by $j_i...j_n,J,m_J$ where only the j_i of the not completely filled subshells are to be taken into account.

The energy difference for larger atoms when placed in a magnetic field is: $\Delta E=g\mu_{\rm B}m_JB$ where g is the Landé factor. For a transition between two singlet states the line splits in 3 parts, for $\Delta m_J=-1,0+1$. This results in the normal Zeeman effect. At higher S the line splits up in more parts: the anomalous Zeeman effect.

Interaction with the spin of the nucleus gives the hyperfine structure.

10.12.4 Selection rules

For the dipole transition matrix elements follows: $p_0\sim|\langle l_2m_2|\vec{E}\cdot\vec{r}\,|l_1m_1\rangle|$. Conservation of angular momentum demands that for the transiting electron holds that $\Delta l=\pm1$.

For an atom where $L-S$ coupling is dominant further holds: $\Delta S=0$ (but not strict), $\Delta L=0,\pm1$, $\Delta J=0,\pm1$ except for $J=0\rightarrow J=0$ transitions, $\Delta m_J=0,\pm1$, but $\Delta m_J=0$ is forbidden if $\Delta J=0$.

For an atom where $j-j$ coupling is dominant further holds: for the jumping electron holds, except $\Delta l=\pm1$, also: $\Delta j=0,\pm1$, and for all other electrons: $\Delta j=0$. For the total atom holds: $\Delta J=0,\pm1$ but no $J=0\rightarrow J=0$ transitions and $\Delta m_J=0,\pm1$, but $\Delta m_J=0$ is forbidden if $\Delta J=0$.

10.13 Interaction with electromagnetic fields

The Hamiltonian of an electron in an electromagnetic field is given by:

$$H=\frac{1}{2\mu}(\vec{p}+e\vec{A})^2-eV=-\frac{\hbar^2}{2\mu}\nabla^2+\frac{e}{2\mu}\vec{B}\cdot\vec{L}+\frac{e^2}{2\mu}A^2-eV$$

where μ is the reduced mass of the system. The term $\sim A^2$ can usually be neglected, except for very strong fields or macroscopic motions. For $\vec{B}=B\vec{e}_z$ it is given by $e^2B^2(x^2+y^2)/8\mu$.

When a gauge transformation $\vec{A'}=\vec{A}-\nabla f$, $V'=V+\partial f/\partial t$ is applied on the potentials the wavefunction is also transformed according to $\psi'=\psi{\rm e}^{iqef/\hbar}$ with qe the charge of the particle. Because $f=f(x,t)$, this is called a *local* gauge transformation, in contrast with a *global* gauge transform which can always be applied.

10.14 Perturbation theory

10.14.1 Time-independent perturbation theory

To solve the equation $(H_0+\lambda H_1)\psi_n=E_n\psi_n$ one has to find the eigenfunctions of $H=H_0+\lambda H_1$. Suppose that ϕ_n is a complete set eigenfunctions is of the nun-perturbed Hamiltonian H_0: $H_0\phi_n=E_n^0\phi_n$. Because ϕ_n is a complete set holds:

$$\psi_n=N(\lambda)\left\{\phi_n+\sum_{k\neq n}c_{nk}(\lambda)\phi_k\right\}$$

When c_{nk} and E_n are being developed to λ: $c_{nk}=\lambda c_{nk}^{(1)}+\lambda^2c_{nk}^{(2)}+\cdots$

$E_n=E_n^0+\lambda E_n^{(1)}+\lambda^2E_n^{(2)}+\cdots$

and this is put into the Schrödinger equation the result is: $E_n^{(1)} = \langle\phi_n|H_1|\phi_n\rangle$ and $c_{nm}^{(1)} = \dfrac{\langle\phi_m|H_1|\phi_n\rangle}{E_n^0 - E_m^0}$ if $m \neq n$. The second-order correction to the energy is than given by: $E_n^{(2)} = \sum\limits_{k\neq n} \dfrac{|\langle\phi_k|H_1|\phi_n\rangle|^2}{E_n^0 - E_k^0}$. So in first order holds: $\psi_n = \phi_n + \sum\limits_{k\neq n} \dfrac{\langle\phi_k|\lambda H_1|\phi_n\rangle}{E_n^0 - E_k^0}\,\phi_k$.

In case the levels are degenerated the above does not hold. In that case an orthonormal set eigenfunctions ϕ_{ni} is chosen for each level n, so that $\langle\phi_{mi}|\phi_{nj}\rangle = \delta_{mn}\delta_{ij}$. Now ψ is developed as:

$$\psi_n = N(\lambda)\left\{\sum_i \alpha_i\phi_{ni} + \lambda\sum_{k\neq n} c_{nk}^{(1)} \sum_i \beta_i\phi_{ki} + \cdots\right\}$$

$E_{ni} = E_{ni}^0 + \lambda E_{ni}^{(1)}$ is approximated by $E_{ni}^0 := E_n^0$. Substitution in the Schrödinger equation and taking dot product with ϕ_{ni} gives: $\sum\limits_i \alpha_i \langle\phi_{nj}|H_1|\phi_{ni}\rangle = E_n^{(1)}\alpha_j$. Norming requires that $\sum\limits_i |\alpha_i|^2 = 1$.

10.14.2 Time-dependent perturbation theory

From the Schrödinger equation $i\hbar\dfrac{\partial\psi(t)}{\partial t} = (H_0 + \lambda V(t))\psi(t)$

and the development $\psi(t) = \sum\limits_n c_n(t)\exp\left(\dfrac{-iE_n^0 t}{\hbar}\right)\phi_n$ with $c_n(t) = \delta_{nk} + \lambda c_n^{(1)}(t) + \cdots$

follows: $c_n^{(1)}(t) = \dfrac{\lambda}{i\hbar}\displaystyle\int\limits_0^t \langle\phi_n|V(t')|\phi_k\rangle \exp\left(\dfrac{i(E_n^0 - E_k^0)t'}{\hbar}\right) dt'$

10.15 N-particle systems

10.15.1 General

Identical particles are indistinguishable. For the total wavefunction of a system of identical indistinguishable particles holds:

1. Particles with a half-odd integer spin (Fermions): $\psi_{\rm total}$ must be antisymmetric w.r.t. interchange of the coordinates (spatial and spin) of each pair of particles. The Pauli principle results from this: two Fermions can not exist in an identical state because then $\psi_{\rm total} = 0$.
2. Particles with an integer spin (Bosons): $\psi_{\rm total}$ must be symmetric w.r.t. interchange of the coordinates (spatial and spin) of each pair of particles.

For a system of two electrons there are 2 possibilities for the spatial wavefunction. When a and b are the quantum numbers of electron 1 and 2 holds:

$$\psi_{\rm S}(1,2) = \psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1) \quad , \quad \psi_{\rm A}(1,2) = \psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)$$

Because the particles do not approach each other closely at $\psi_{\rm A}$ the repulsion energy in this state is smaller. The following spin wavefunctions are possible:

$$\chi_{\rm A} = \tfrac{1}{2}\sqrt{2}[\chi_+(1)\chi_-(2) - \chi_+(2)\chi_-(1)] \quad m_s = 0$$

$$\chi_{\rm S} = \left\{\begin{array}{ll} \chi_+(1)\chi_+(2) & m_s = +1 \\ \tfrac{1}{2}\sqrt{2}[\chi_+(1)\chi_-(2) + \chi_+(2)\chi_-(1)] & m_s = 0 \\ \chi_-(1)\chi_-(2) & m_s = -1 \end{array}\right.$$

Because the total wavefunction must be antisymmetric follows: $\psi_{\rm total} = \psi_{\rm S}\chi_{\rm A}$ óf $\psi_{\rm total} = \psi_{\rm A}\chi_{\rm S}$.

For N particles the symmetric spatial function is given by:

$$\psi_{\rm S}(1,...,N)=\sum\psi(\text{all permutations of }1..N)$$

The antisymmetric wavefunction is given by the determinant $\psi_{\rm A}(1,...,N)=\dfrac{1}{\sqrt{N!}}|u_{E_i}(j)|$

10.15.2 Molecules

The wavefunctions of atom a and b are ϕ_a and ϕ_b. If the 2 atoms approach each other there are two possibilities: the total wavefunction approaches the bonding function with lower total energy $\psi_{\rm B}=\frac{1}{2}\sqrt{2}(\phi_a+\phi_b)$ or approaches the anti-bonding function with higher energy $\psi_{\rm AB}=\frac{1}{2}\sqrt{2}(\phi_a-\phi_b)$. If a molecular-orbital is symmetric w.r.t. the connecting axis, like a combination of two s-orbitals it is called a σ-orbital, otherwise a π-orbital, like the combination of two p-orbitals along two axes.

The energy of a system is: $E=\dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$.

The energy calculated with this method is always *higher* than the real energy if ψ is only an approximation for the solutions of $H\psi=E\psi$. Also, if there can be chosen of more functions, the function which gives the lowest energy is the best approximation. Applying this on the function $\psi=\sum c_i\phi_i$ one finds: $(H_{ij}-ES_{ij})c_i=0$. This equation has only solutions if the *secular determinant* $|H_{ij}-ES_{ij}|=0$. Here, $H_{ij}=\langle\phi_i|H|\phi_j\rangle$ and $S_{ij}=\langle\phi_i|\phi_j\rangle$. $\alpha_i:=H_{ii}$ is the Coulomb integral and $\beta_{ij}:=H_{ij}$ the exchange integral. $S_{ii}=1$ and S_{ij} is the overlap integral.

The first approximation in the molecular-orbital theory is to place both electrons of a chemical bond in the bonding orbital: $\psi(1,2)=\psi_{\rm B}(1)\psi_{\rm B}(2)$. This results in a large electron density between the nuclei and therefore a repulsion. A better approximation is: $\psi(1,2)=C_1\psi_{\rm B}(1)\psi_{\rm B}(2)+C_2\psi_{\rm AB}(1)\psi_{\rm AB}(2)$, with $C_1=1$ and $C_2\approx 0,6$.

In some atoms, like C, it is energetical more suitable to form orbitals which are a linear combination of the s, p and d states. There are three ways of hybridization in C:

1. SP-hybridization: $\psi_{\rm sp}=\frac{1}{2}\sqrt{2}(\psi_{\rm 2s}\pm\psi_{{\rm 2p}_z})$. There are 2 hybrid orbitals who are placed at one line under 180°. Further the 2p$_x$ and 2p$_y$ orbitals remain.
2. SP^2 hybridization: $\psi_{{\rm sp}^2}=\psi_{\rm 2s}+c_1\psi_{{\rm 2p}_z}+c_2\psi_{{\rm 2p}_y}$, where $(c_1,c_2)\in\{(1,-1,0),(1,1,-1),(1,1,1)\}$. The 3 SP^2 orbitals lay in one plane, their symmetry axes who are at an angle of 120°.
3. SP^3 hybridization: $\psi_{{\rm sp}^3}=\frac{1}{2}(\psi_{\rm 2s}\pm\psi_{{\rm 2p}_z}\pm\psi_{{\rm 2p}_y}\pm\psi_{{\rm 2p}_x})$. The 4 SP^3 orbitals form a tetraheder with the symmetry axes at an angle of $109^\circ 28'$.

10.16 Quantum statistics

If a system exists in a state in which one has not the maximal amount of information about the system, it can be described with a *density matrix* ρ. If the probability that the system is in state ψ_i is given by a_i, one can write for the expectation value a of A: $\langle a\rangle=\sum\limits_i r_i\langle\psi_i|A|\psi_i\rangle$.

If ψ is developed to an orthonormal basis $\{\phi_k\}$ as: $\psi^{(i)}=\sum\limits_k c_k^{(i)}\phi_k$, holds:

$$\langle A\rangle=\sum_k(A\rho)_{kk}={\rm Tr}(A\rho)$$

where $\rho_{lk}=c_k^*c_l$. ρ is hermitian, with ${\rm Tr}(\rho)=1$. Further holds $\rho=\sum r_i|\psi_i\rangle\langle\psi_i|$. The probability to find eigenvalue a_n when measuring A is given by ρ_{nn} if one uses a basis of eigenvectors of A for $\{\phi_k\}$. For the time-dependence holds (in the Schrödinger image operators are not explicitly time-dependent):

$$i\hbar\frac{d\rho}{dt}=[H,\rho]$$

For a macroscopic system in equilibrium holds $[H,\rho]=0$. If all quantumstates with the same energy are equally probable: $P_i=P(E_i)$, one can obtain the distribution:

$$P_n(E)=\rho_{nn}=\frac{\mathrm{e}^{-E_n/kT}}{Z}\ \ \text{with the state sum}\ \ Z=\sum_n \mathrm{e}^{-E_n/kT}$$

The thermodynamic quantities are related with these definitions as follows: $F=-kT\ln(Z)$, $U=\langle H\rangle=\sum\limits_n p_nE_n=-\dfrac{\partial}{\partial kT}\ln(Z)$, $S=-k\sum\limits_n P_n\ln(P_n)$. For a mixed state of M orthonormal quantum states with probability $1/M$ follows: $S=k\ln(M)$.

The distribution function for the internal states for a system in thermic equilibrium is the most probable function. This function can be found by finding the maximum of the function which gives the number of states with Stirling's equation: $\ln(n!)\approx n\ln(n)-n$, and the conditions $\sum\limits_k n_k=N$ and $\sum\limits_k n_kW_k=W$. For identical, indistinguishable particles who obey the Pauli exclusion principle the possible number of states is given by:

$$P=\prod_k\frac{g_k!}{n_k!(g_k-n_k)!}$$

This results in the *Fermi-Dirac statistics*. For indistinguishable particles who *do not* obey the exclusion principle the possible number of states is given by:

$$P=N!\prod_k\frac{g_k^{n_k}}{n_k!}$$

This results in the *Bose-Einstein statistics*. So the distribution functions who explain how particles are distributed over the different one-particle states k who are each g_k-fold degenerate depend on the spin of the particles. They are given by:

1. Fermi-Dirac statistics: integer spin. $n_k\in\{0,1\}$, $n_k=\dfrac{N}{Z_g}\dfrac{g_k}{\exp((E_k-\mu)/kT)+1}$ with $\ln(Z_{\rm g})=\sum g_k\ln[1+\exp((E_i-\mu)/kT)]$.
2. Bose-Einstein statistics: half odd-integer spin. $n_k\in I\!N$, $n_k=\dfrac{N}{Z_g}\dfrac{g_k}{\exp((E_k-\mu)/kT)-1}$ with $\ln(Z_{\rm g})=-\sum g_k\ln[1-\exp((E_i-\mu)/kT)]$.

Here, $Z_{\rm g}$ is the large-canonical state sum and μ the chemical potential. It is found by demanding $\sum n_k=N$, and for it holds: $\lim\limits_{T\rightarrow0}\mu=E_{\rm F}$, the Fermi-energy. N is the total number of particles. The Maxwell-Boltzmann distribution can be derived from this in the limit $E_k-\mu\gg kT$:

$$n_k=\frac{N}{Z}\exp\left(-\frac{E_k}{kT}\right)\ \ \text{with}\ \ Z=\sum_k g_k\exp\left(-\frac{E_k}{kT}\right)$$

With the Fermi-energy, the Fermi-Dirac and Bose-Einstein statistics can be written as:

1. Fermi-Dirac statistics: $n_k=\dfrac{g_k}{\exp((E_k-E_{\rm F})/kT)+1}$.
2. Bose-Einstein statistics: $n_k=\dfrac{g_k}{\exp((E_k-E_{\rm F})/kT)-1}$.

Chapter 11

Plasma physics

11.1 Introduction

The *degree of ionization* α of a plasma is defined by: $\alpha = \dfrac{n_\mathrm{e}}{n_\mathrm{e} + n_0}$

where n_e is the electron density and n_0 the density of the neutrals. If a plasma contains also negative charged ions α is not well defined.

The probability that a test particle has a collision with another is given by $dP = n\sigma dx$ where σ is the *cross section*. The collision frequency $\nu_\mathrm{c} = 1/\tau_\mathrm{c} = n\sigma v$. The *mean free path* is given by $\lambda_\mathrm{v} = 1/n\sigma$. The *ratecoefficient* K is defined by $K = \langle \sigma v \rangle$. The number of collisions per unit of time and volume between particles of kind 1 and 2 is given by $n_1 n_2 \langle \sigma v \rangle = K n_1 n_2$.

The potential of an electron is given by:

$$V(r) = \frac{-e}{4\pi\varepsilon_0 r} \exp\left(-\frac{r}{\lambda_\mathrm{D}}\right) \quad \text{with} \quad \lambda_\mathrm{D} = \sqrt{\frac{\varepsilon_0 k T_\mathrm{e} T_\mathrm{i}}{e^2(n_\mathrm{e} T_\mathrm{i} + n_\mathrm{i} T_\mathrm{e})}} \approx \sqrt{\frac{\varepsilon_0 k T_\mathrm{e}}{n_\mathrm{e} e^2}}$$

because charge is shielded in a plasma. Here, λ_D is the *Debye length*. For distances $< \lambda_\mathrm{D}$ the plasma can not be assumed to be quasi-neutral. Deviations of charge neutrality by thermic motion are compensated by oscillations with frequency

$$\omega_\mathrm{pe} = \sqrt{\frac{n_\mathrm{e} e^2}{m_\mathrm{e} \varepsilon_0}}$$

The distance of closest approximation when two equal charged particles collide for a deviation of $\pi/2$ is $2b_0 = e^2/(4\pi\varepsilon_0 \frac{1}{2} m v^2)$. A "neat" plasma is defined as a plasma for which holds: $b_0 < n_\mathrm{e}^{-1/3} \ll \lambda_\mathrm{D} \ll L_\mathrm{p}$. Here $L_\mathrm{p} := |n_\mathrm{e}/\nabla n_\mathrm{e}|$ is the gradient length of the plasma.

11.2 Transport

Relaxation times are defined as $\tau = 1/\nu_\mathrm{c}$. Starting with $\sigma_\mathrm{m} = 4\pi b_0^2 \ln(\Lambda_\mathrm{C})$ and with $\frac{1}{2} m v^2 = kT$ it can be found that:

$$\tau_\mathrm{m} = \frac{4\pi\varepsilon_0^2 m^2 v^3}{n e^4 \ln(\Lambda_\mathrm{C})} = \frac{8\sqrt{2}\pi\varepsilon_0^2 \sqrt{m}(kT)^{3/2}}{n e^4 \ln(\Lambda_\mathrm{C})}$$

For momentum transfer between electrons and ions holds for a Maxwellian velocity distribution:

$$\tau_\mathrm{ee} = \frac{6\pi\sqrt{3}\varepsilon_0^2 \sqrt{m_\mathrm{e}}(kT_\mathrm{e})^{3/2}}{n_\mathrm{e} e^4 \ln(\Lambda_\mathrm{C})} \approx \tau_\mathrm{ei} \quad , \quad \tau_\mathrm{ii} = \frac{6\pi\sqrt{3}\varepsilon_0^2 \sqrt{m_\mathrm{i}}(kT_\mathrm{i})^{3/2}}{n_\mathrm{i} e^4 \ln(\Lambda_\mathrm{C})}$$

The energy relaxation times for equal particles are equal to the momentum relaxation times. Because for e-i collisions the energy transfer is only $\sim 2m_\mathrm{e}/m_\mathrm{i}$ this is a slow process. Approximately holds: $\tau_\mathrm{ee} : \tau_\mathrm{ei} : \tau_\mathrm{ie} : \tau_\mathrm{ie}^E = 1 : 1 : \sqrt{m_\mathrm{i}/m_\mathrm{e}} : m_\mathrm{i}/m_\mathrm{e}$.

The relaxation for e-o interaction is much more complicated. For $T > 10$ eV holds approximately: $\sigma_\mathrm{eo} = 10^{-17} v_\mathrm{e}^{-2/5}$, for lower energies this can be a factor 10 lower.

The resistivity $\eta = E/J$ of a plasma is given by:

$$\eta = \frac{n_{\rm e}e^2}{m_{\rm e}\nu_{\rm ei}} = \frac{e^2\sqrt{m_{\rm e}}\ln(\Lambda_{\rm C})}{6\pi\sqrt{3}\varepsilon_0^2(kT_{\rm e})^{3/2}}$$

The diffusion coefficient D is defined via the flux Γ by $\vec{\Gamma} = n\vec{v}_{\rm diff} = -D\nabla n$. The equation of continuity is $\partial_t n + \nabla(nv_{\rm diff}) = 0 \Rightarrow \partial_t n = D\nabla^2 n$. One finds that $D = \frac{1}{3}\lambda_{\rm v}v$. A rough estimate gives $\tau_{\rm D} = L_{\rm p}/D = L_{\rm p}^2\tau_{\rm c}/\lambda_{\rm v}^2$. For magnetized plasma's $\lambda_{\rm v}$ must be replaced with the cyclotron radius. In electrical fields also holds $\vec{J} = ne\mu\vec{E} = e(n_{\rm e}\mu_{\rm e} + n_{\rm i}\mu_{\rm i})\vec{E}$ with $\mu = e/m\nu_{\rm c}$ the mobility of the particles. The Einstein ratio is:

$$\frac{D}{\mu} = \frac{kT}{e}$$

Because a plasma is electrical neutral electrons and ions are strongly coupled and they don't diffuse independent. The *coefficient of ambipolar diffusion* $D_{\rm amb}$ is defined by $\vec{\Gamma} = \vec{\Gamma}_{\rm i} = \vec{\Gamma}_{\rm e} = -D_{\rm amb}\nabla n_{\rm e,i}$. From this follows that

$$D_{\rm amb} = \frac{kT_{\rm e}/e - kT_{\rm i}/e}{1/\mu_{\rm e} - 1/\mu_{\rm i}} \approx \frac{kT_{\rm e}\mu_{\rm i}}{e}$$

In an external magnetic field B_0 particles will move in spiral orbits with *cyclotron radius* $\rho = mv/eB_0$ and with cyclotron frequency $\Omega = B_0e/m$. The spiralized orbit is disturbed by collisions. A plasma is called *magnetized* if $\lambda_{\rm v} > \rho_{\rm e,i}$. So the electrons are magnetized if

$$\frac{\rho_{\rm e}}{\lambda_{\rm ee}} = \frac{\sqrt{m_{\rm e}}e^3n_{\rm e}\ln(\Lambda_{\rm C})}{6\pi\sqrt{3}\varepsilon_0^2(kT_{\rm e})^{3/2}B_0} < 1$$

Magnetization of only the electrons is sufficient to confine the plasma reasonable because they are coupled to the ions by charge neutrality. In case of magnetic confinement holds: $\nabla p = \vec{J} \times \vec{B}$. Combined with the two stationary Maxwell equations for the B-field these form the ideal magneto-hydrodynamic equations. For a uniform B-field holds: $p = nkT = B^2/2\mu_0$.

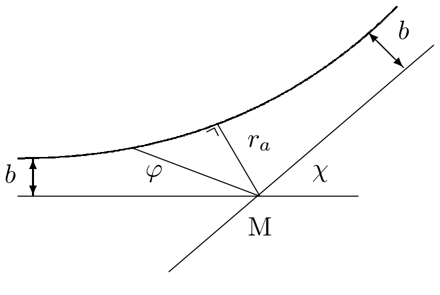
If both magnetic and electric fields are present electrons and ions will move in the same direction. If $\vec{E} = E_r\vec{e}_r + E_z\vec{e}_z$ and $\vec{B} = B_z\vec{e}_z$ the $\vec{E} \times \vec{B}$ drift results in a velocity $\vec{u} = (\vec{E} \times \vec{B})/B^2$ and the velocity in the r,φ plane is $\dot{r}(r,\varphi,t) = \vec{u} + \dot{\vec{\rho}}(t)$.

11.3 Elastic collisions

11.3.1 General

The scattering angle of a particle in interaction with another particle, as shown in the figure at the right is:

$$\chi = \pi - 2b\int\limits_{r_a}^{\infty}\frac{dr}{r^2\sqrt{1 - \dfrac{b^2}{r^2} - \dfrac{W(r)}{E_0}}}$$



Particles with an impact parameter between b and $b + db$, going through a ring with $d\sigma = 2\pi b db$ leave the scattering area at a solid angle $d\Omega = 2\pi\sin(\chi)d\chi$. The *differential cross section* is then defined as:

$$I(\Omega) = \left|\frac{d\sigma}{d\Omega}\right| = \frac{b}{\sin(\chi)}\frac{\partial b}{\partial\chi}$$

For a potential energy $W(r) = kr^{-n}$ follows: $I(\Omega, v) \sim v^{-4/n}$.

For low energies, $\mathcal{O}(1 \text{ eV})$, σ has a *Ramsauer minimum.* It arises from the interference of matter waves behind the object. $I(\Omega)$ for angles $0 < \chi < \lambda/4$ is larger than the classical value.

11.3.2 The Coulomb interaction

For the Coulomb interaction holds: $2b_0 = q_1q_2/2\pi\varepsilon_0 mv_0^2$, so $W(r) = 2b_0/r$. This gives $b = b_0\cot(\frac{1}{2}\chi)$ and

$$I(\Omega = \frac{b}{\sin(\chi)}\frac{\partial b}{\partial \chi} = \frac{b_0^2}{4\sin^2(\frac{1}{2}\chi)}$$

Because the influence of a particle vanishes at $r = \lambda_{\rm D}$ holds: $\sigma = \pi(\lambda_{\rm D}^2 - b_0^2)$. Because $dp = d(mv) = mv_0(1-\cos\chi)$ a cross section related to momentum transfer $\sigma_{\rm m}$ is given by:

$$\sigma_{\rm m} = \int (1-\cos\chi) I(\Omega)d\Omega = 4\pi b_0^2 \ln\left(\frac{1}{\sin(\frac{1}{2}\chi_{\rm min})}\right) = 4\pi b_0^2 \ln\left(\frac{\lambda_{\rm D}}{b_0}\right) := 4\pi b_0^2\ln(\Lambda_{\rm C}) \sim \frac{\ln(v^4)}{v^4}$$

where $\ln(\Lambda_{\rm C})$ is the *Coulomb-logarithm*. For this quantity holds: $\Lambda_{\rm C} = \lambda_{\rm D}/b_0 = 9n(\lambda_{\rm D})$.

11.3.3 The induced dipole interaction

The induced dipole interaction, with $\vec{p} = \alpha\vec{E}$, gives a potential V and an energy W in a dipole field given by:

$$V(r) = \frac{\vec{p}\cdot\vec{e}_r}{4\pi\varepsilon_0 r^2} \ \ , \ \ W(r) = -\frac{|e|p}{8\pi\varepsilon_0 r^2} = -\frac{\alpha e^2}{2(4\pi\varepsilon_0)^2 r^4}$$

with $b_a = \sqrt[4]{\dfrac{2e^2\alpha}{(4\pi\varepsilon_0)^2\frac{1}{2}mv_0^2}}$ holds: $\chi = \pi - 2b\displaystyle\int_{r_a}^{\infty}\frac{dr}{r^2\sqrt{1 - \dfrac{b^2}{r^2} + \dfrac{b_a^4}{4r^4}}}$

If $b \geq b_a$ the charge would hit the atom. Repulsing nuclear forces prevent this to happen. If the scattering angle is many times 2π it is called capture. The cross section for capture $\sigma_{\rm orb} = \pi b_a^2$ is called the Langevin limit, and is a lowest estimate for the total cross section.

11.3.4 The center of mass system

If collisions of two particles with masses m_1 and m_2 who scatter in the center of mass system under an angle χ are compared with the scattering under an angle θ in the laboratory system holds:

$$\tan(\theta) = \frac{m_2\sin(\chi)}{m_1 + m_2\cos(\chi)}$$

The energy loss ΔE of the incoming particle is given by:

$$\frac{\Delta E}{E} = \frac{\frac{1}{2}m_2v_2^2}{\frac{1}{2}m_1v_1^2} = \frac{2m_1m_2}{(m_1+m_2)^2}(1-\cos(\chi))$$

11.3.5 Scattering of light at free electrons

Scattering of light at free electrons is called Thomson scattering. The scattering is free of collective effects if $k\lambda_{\rm D} \ll 1$. The cross section $\sigma = 6{,}65\cdot 10^{-29}{\rm m}^2$ and

$$\frac{\Delta f}{f} = \frac{2v}{c}\sin(\tfrac{1}{2}\chi)$$

This gives for the scattered energy $E_{\rm scat} = N\lambda_0^4/(\lambda^2 - \lambda_0^2)^2$. If relativistic effects become important, this limit of Compton scattering (which is given by $\lambda' - \lambda = \lambda_{\rm C}(1-\cos\chi)$ with $\lambda_{\rm C} = h/mc$) can not be used any more.

11.4 Thermodynamic equilibrium and reversibility

For a plasma in equilibrium holds Planck's radiation law and the Maxwellian velocity distribution:

$$\rho(\nu,T)d\nu=\frac{8\pi h\nu^3}{c^3}\frac{1}{\exp(h\nu/kT)-1}d\nu \quad , \quad N(E,T)dE=\frac{2\pi n}{(\pi kT)^{3/2}}\sqrt{E}\exp\left(-\frac{E}{kT}\right)dE$$

"Detailed balancing" means that the number of reactions in one direction equals the number of reactions in the opposite direction because both processes have equal probability if one corrects for the used phase space. For the reaction

$$\sum_{\text{forward}}\mathrm{X}_{\text{forward}} \rightleftarrows \sum_{\text{back}}\mathrm{X}_{\text{back}}$$

holds in a plasma in equilibrium *microscopic* reversibility:

$$\prod_{\text{forward}}\hat{\eta}_{\text{forward}}=\prod_{\text{back}}\hat{\eta}_{\text{back}}$$

If the velocity distribution is Maxwellian, this gives:

$$\hat{\eta}_x=\frac{n_x}{g_x}\frac{h^3}{(2\pi m_x kT)^{3/2}}\mathrm{e}^{-E_{\text{kin}}/kT}$$

where g is the statistical weight of the state and $n/g := \eta$. For electrons holds $g=2$, for excited states usually holds $g=2j+1=2n^2$.

With this one finds for the Boltzmann balance: $\mathrm{X}_p+\mathrm{e}^- \rightleftarrows \mathrm{X}_1+\mathrm{e}^-+(E_{1p})$:

$$\frac{n_p}{n_1}=\frac{g_p}{g_1}\exp\left(\frac{E_p-E_1}{kT_{\mathrm{e}}}\right)$$

And for the Saha balance: $\mathrm{X}_p+\mathrm{e}^-+(E_{pi}) \rightleftarrows \mathrm{X}_1^+ +2\mathrm{e}^-$:

$$\frac{n_p^{\mathrm{S}}}{g_p}=\frac{n_1^+}{g_1^+}\frac{n_{\mathrm{e}}}{g_{\mathrm{e}}}\frac{h^3}{(2\pi m_{\mathrm{e}}kT_{\mathrm{e}})^{3/2}}\exp\left(\frac{E_{pi}}{kT_{\mathrm{e}}}\right)$$

Because the number of particles on the left-hand side and right-hand side of the equation is different, a factor g/V_{e} remains. This factor causes the Saha-jump.

From microscopic reversibility one can derive that for the rate coefficients $K(p,q,T):=\langle\sigma v\rangle_{pq}$ holds:

$$K(q,p,T)=\frac{g_p}{g_q}K(p,q,T)\exp\left(\frac{\Delta E_{pq}}{kT}\right)$$

11.5 Inelastic collisions

11.5.1 Types of collisions

The kinetic energy can be split in a part *of* and a part *in* the center of mass system. The energy *in* the center of mass system is available for reactions. This energy is given by

$$E=\frac{m_1m_2(v_1-v_2)^2}{2(m_1+m_2)}$$

Some types of inelastic collisions important for plasma physics are:

1. Excitation: $\mathrm{A}_p+\mathrm{e}^- \rightleftarrows \mathrm{A}_q+\mathrm{e}^-$
2. Decay: $\mathrm{A}_q \rightleftarrows \mathrm{A}_p+hf$

3. Ionisation and 3-particles recombination: $\mathrm{A}_p + \mathrm{e}^- \rightleftarrows \mathrm{A}^+ + 2\mathrm{e}^-$
4. radiative recombination: $\mathrm{A}^+ + \mathrm{e}^- \rightleftarrows \mathrm{A}_p + hf$
5. Stimulated emission: $\mathrm{A}_q + hf \rightarrow \mathrm{A}_p + 2hf$
6. Associative ionisation: $\mathrm{A}^{**} + \mathrm{B} \rightleftarrows \mathrm{AB}^+ + \mathrm{e}^-$
7. Penning ionisation: b.v. $\mathrm{Ne}^* + \mathrm{Ar} \rightleftarrows \mathrm{Ar}^+ + \mathrm{Ne} + \mathrm{e}^-$
8. Charge transfer: $\mathrm{A}^+ + \mathrm{B} \rightleftarrows \mathrm{A} + \mathrm{B}^+$
9. Resonant charge transfer: $\mathrm{A}^+ + \mathrm{A} \rightleftarrows \mathrm{A} + \mathrm{A}^+$

11.5.2 Cross sections

Collisions between an electron and an atom can be approximated by a collision between an electron and one of the electrons of that atom. This results in

$$\frac{d\sigma}{d(\Delta E)} = \frac{\pi Z^2 e^4}{(4\pi\varepsilon_0)^2 E(\Delta E)^2}$$

Then follows for the transition $p \rightarrow q$: $\sigma_{pq}(E) = \dfrac{\pi Z^2 e^4 \Delta E_{q,q+1}}{(4\pi\varepsilon_0)^2 E(\Delta E)^2_{pq}}$

For ionisation from state p holds in good approximation: $\sigma_p = 4\pi a_0^2 Ry \left(\dfrac{1}{E_p} - \dfrac{1}{E}\right) \ln\left(\dfrac{1,25\beta E}{E_p}\right)$

For resonant charge transfer holds: $\sigma_{\rm ex} = \dfrac{A[1 - B\ln(E)]^2}{1 + CE^{3,3}}$

11.6 Radiation

In equilibrium holds for radiation processes:

$$\underbrace{n_p A_{pq}}_{\text{emission}} + \underbrace{n_p B_{pq}\rho(\nu,T)}_{\text{stimulated emission}} = \underbrace{n_q B_{qp}\rho(\nu,T)}_{\text{absorption}}$$

Here, A_{pq} is the matrix element of the transition $p \rightarrow q$, and is given by:

$$A_{pq} = \frac{8\pi^2 e^2 \nu^3 |r_{pq}|^2}{3\hbar\varepsilon_0 c^3} \quad \text{with} \quad r_{pq} = \langle\psi_p|\vec{r}\ |\psi_q\rangle$$

For hydrogen-like atoms holds: $A_p = 1,58\cdot 10^8 Z^4 p^{-4,5}$, with $A_p = 1/\tau_p = \sum\limits_q A_{pq}$. The intensity I af a line is given by $I_{pq} = hfA_{pq}n_p/4\pi$. The Einstein coefficients B are given by:

$$B_{pq} = \frac{c^3 A_{pq}}{8\pi h\nu^3} \quad \text{en} \quad \frac{B_{pq}}{B_{qp}} = \frac{g_q}{g_p}$$

A spectral line is broadened by several mechanisms:

1. Because the states have a finite life time. The natural life time of a state p is given by $\tau_p = 1/\sum\limits_q A_{pq}$. From the uncertaincy relation then follows: $\Delta(h\nu)\cdot\tau_p = \frac{1}{2}\hbar$, this gives

$$\Delta\nu = \frac{1}{4\pi\tau_p} = \frac{\sum\limits_q A_{pq}}{4\pi}$$

The natural line width is usually $\ll$ than the broadening from the following two mechanisms:

2. The Doppler broadening is caused by the thermic motion of the particles:

   $$\frac{\Delta\lambda}{\lambda}=\frac{2}{c}\sqrt{\frac{2\ln(2kT_{\rm i})}{m_{\rm i}}}$$

   This broadening results in a Gaussian line profile:
   $k_\nu=k_0\exp(-[2\sqrt{\ln 2}(\nu-\nu_0)/\Delta\nu_D]^2)$, with k the coefficient of absorption or emission.

3. The Stark broadening is caused by the electric fields of the electrons:

   $$\Delta\lambda_{1/2}=\left[\frac{n_{\rm e}}{C(n_{\rm e},T_{\rm e})}\right]^{2/3}$$

   with for the H-β line: $C(n_{\rm e},T_{\rm e})\approx 3\cdot 10^{14}\text{Å}^{-3/2}\text{cm}^{-3}$.

The natural broadening and the Stark broadening result in a Lorentz profile of a spectral line: $k_\nu=\frac{1}{2}k_0\Delta\nu_L/[(\frac{1}{2}\Delta\nu_L)^2+(\nu-\nu_0)^2]$. The total line shape is a convolution of the Gauss- and Lorentz profile and is called a *Voigt profile.*

The number of transitions $p\rightarrow q$ is given by $n_pB_{pq}\rho$ and by $n_pn_{hf}\langle\sigma_{\rm a}c\rangle=n_p(\rho d\nu/h\nu)\sigma_{\rm a}c$ where $d\nu$ is the line width. Then follows for the cross section of absorption processes: $\sigma_{\rm a}=B_{pq}h\nu/cd\nu$.

The background radiation in a plasma originates from two processes:

1. Free-Bound radiation, originating from radiative recombination. The emission is given by:

   $$\varepsilon_{fb}=\frac{C_1}{\lambda^2}\frac{z_{\rm i}n_{\rm i}n_{\rm e}}{\sqrt{kT_{\rm e}}}\left[1-\exp\left(-\frac{hc}{\lambda kT_{\rm e}}\right)\right]\xi_{fb}(\lambda,T_{\rm e})$$

   with $C_1=1,63\cdot 10^{-43}$ $\text{Wm}^4\text{K}^{1/2}\text{sr}^{-1}$ and ξ the *Biberman factor.*

2. Free-free radiation, originating from the acceleration of particles in the EM-field of other particles:

   $$\varepsilon_{ff}=\frac{C_1}{\lambda^2}\frac{z_{\rm i}n_{\rm i}n_{\rm e}}{\sqrt{kT_{\rm e}}}\exp\left(-\frac{hc}{\lambda kT_{\rm e}}\right)\xi_{ff}(\lambda,T_{\rm e})$$

11.7 The Boltzmann transport equation

It is assumed that there exist a distribution function F for the plasma so that

$$F(\vec{r},\vec{v},t)=F_r(\vec{r},t)\cdot F_v(\vec{v},t)=F_1(x,t)F_2(y,t)F_3(z,t)F_4(v_x,t)F_5(v_y,t)F_6(v_z,t)$$

Then the BTE is: $\displaystyle\frac{dF}{dt}=\frac{\partial F}{\partial t}+\nabla_r\cdot(F\vec{v})+\nabla_v\cdot(F\vec{a})=\left(\frac{\partial F}{\partial t}\right)_{\rm coll-rad}$

Assuming that v does not depends on r and a_i not depends on v_i, holds $\nabla_r\cdot(F\vec{v})=\vec{v}\cdot\nabla F$ and $\nabla_v\cdot(F\vec{a})=\vec{a}\cdot\nabla_vF$. This is also true in magnetic fields because $\partial a_i/\partial x_i=0$. The velocity is separated in a thermic velocity $\vec{v}_{\rm t}$ and a drift velocity $\vec{w}$. The total density is given by $n=\int Fd\vec{v}$ and $\int\vec{v}Fd\vec{v}=n\vec{w}$.

The balance equations can be derived with the moment method:

1. Mass balance: $\displaystyle\int(\text{BTE})d\vec{v}\Rightarrow\frac{\partial n}{\partial t}+\nabla\cdot(n\vec{w})=\left(\frac{\partial n}{\partial t}\right)_{\rm bs}$

2. Momentum balance: $\displaystyle\int(\text{BTE})m\vec{v}d\vec{v}\Rightarrow mn\frac{d\vec{w}}{dt}+\nabla\mathsf{T}'+\nabla p=mn\langle\vec{a}\ \rangle+\vec{R}$

3. Energy balance: $\displaystyle\int(\text{BTE})mv^2d\vec{v}\Rightarrow\frac{3}{2}\frac{dp}{dt}+\frac{5}{2}p\nabla\cdot\vec{w}+\nabla\cdot\vec{q}=Q$

Here, $\langle \vec{a}\,\rangle = e/m(\vec{E}+\vec{w}\times\vec{B})$ is the average acceleration, $\vec{q}=\frac{1}{2}nm\left\langle \vec{v}_{\rm t}^{\,2}\vec{v}_{\rm t}\right\rangle$ the heat flow, $Q=\displaystyle\int\frac{mv_{\rm t}^2}{r}\left(\frac{\partial F}{\partial t}\right)_{\rm bs}d\vec{v}$ the source term for energy production, $\vec{R}$ is a friction term and $p=nkT$ the pressure.

A thermodynamic derivation gives for the total pressure: $p=nkT=\displaystyle\sum_i p_i-\frac{e^2(n_{\rm e}+z_{\rm i}n_{\rm i})}{24\pi\varepsilon_0\lambda_{\rm D}}$

For the electrical conductance in a plasma follows from the momentum balance, if $w_{\rm e}\gg w_{\rm i}$:

$$\eta\vec{J}=\vec{E}-\frac{\vec{J}\times\vec{B}+\nabla p_{\rm e}}{en_{\rm e}}$$

In a plasma where only elastic e-a collisions are important the equilibrium energy distribution function is the *Druyvesteyn distribution*:

$$N(E)dE=Cn_{\rm e}\left(\frac{E}{E_0}\right)^{3/2}\exp\left[-\frac{3m_{\rm e}}{m_0}\left(\frac{E}{E_0}\right)^2\right]dE$$

with $E_0=eE\lambda_{\rm v}=eE/n\sigma$.

11.8 Collision-radiative models

These models are first-moment equations for excited states. One assumes the Quasi-steady-state solution is valid, where $\forall_{p>1}[(\partial n_p/\partial t=0)\wedge(\nabla\cdot(n_p\vec{w}_p)=0)]$. This results in:

$$\left(\frac{\partial n_{p>1}}{\partial t}\right)_{\rm bs}=0~~,~~\frac{\partial n_1}{\partial t}+\nabla\cdot(n_1\vec{w}_1)=\left(\frac{\partial n_1}{\partial t}\right)_{\rm bs}~~,~~\frac{\partial n_{\rm i}}{\partial t}+\nabla\cdot(n_{\rm i}\vec{w}_{\rm i})=\left(\frac{\partial n_{\rm i}}{\partial t}\right)_{\rm bs}$$

with as solutions $n_p=r_p^0n_p^{\rm S}+r_p^1n_p^{\rm B}=b_pn_p^{\rm S}$. Further holds for all collision-dominated levels that $\delta b_p:=b_p-1=b_0p_{\rm eff}^{-x}$ with $p_{\rm eff}=\sqrt{Ry/E_{p{\rm i}}}$ and $5\leq x\leq 6$. For systems in ESP, where only collisional (de)excitation between levels p and $p\pm 1$ is taken into account holds $x=6$. Even in plasma's far from equilibrium the excited levels will eventually reach ESP, so from a certain level up the level densities can be calculated.

To find the population densities of the lower levels in the stationary case one has to start with a macroscopic equilibrium:

$$\mbox{Number of populating processes of level } p ~=~ \mbox{Number of depopulating processes of level } p~,$$

When this is expanded it becomes:

$$\underbrace{n_{\rm e}\sum_{q<p}n_qK_{qp}}_{\mbox{coll. excit.}}+\underbrace{n_{\rm e}\sum_{q>p}n_qK_{qp}}_{\mbox{coll. deexcit.}}+\underbrace{\sum_{q>p}n_qA_{qp}}_{\mbox{rad. deex. to}}+\underbrace{n_{\rm e}^2n_{\rm i}K_{+p}}_{\mbox{coll. recomb.}}+\underbrace{n_{\rm e}n_{\rm i}\alpha_{\rm rad}}_{\mbox{rad. recomb}}=$$

$$\underbrace{n_{\rm e}n_p\sum_{q<p}K_{pq}}_{\mbox{coll. deexcit.}}+\underbrace{n_{\rm e}n_p\sum_{q>p}K_{pq}}_{\mbox{col. excit.}}+\underbrace{n_p\sum_{q<p}A_{pq}}_{\mbox{rad. deex. from}}+\underbrace{n_{\rm e}n_pK_{p+}}_{\mbox{coll. ion.}}$$

11.9 Waves in plasma's

Interaction of electromagnetic weaves in plasma's results in scattering and absorption of energy. For electromagnetic waves with complex wave number $k=\omega(n+i\kappa)/c$ in one dimension one finds: $E_x=E_0{\rm e}^{-\kappa\omega x/c}\cos[\omega(t-nx/c)]$. The refractive index n is given by:

$$n=c\frac{k}{\omega}=\frac{c}{v_{\rm f}}=\sqrt{1-\frac{\omega_{\rm p}^2}{\omega^2}}$$

For disturbances in the z-direction in a cold, homogeneous, magnetized plasma: $\vec{B}=B_0\vec{e}_z+\vec{\hat{B}}\mathrm{e}^{i(kz-\omega t)}$ and $n=n_0+\hat{n}\mathrm{e}^{i(kz-\omega t)}$ (external E fields are screened) follows, with the definitions $\alpha=\omega_\mathrm{p}/\omega$ and $\beta=\Omega/\omega$ and $\omega_\mathrm{p}^2=\omega_\mathrm{pi}^2+\omega_\mathrm{pe}^2$:

$$\vec{J}=\vec{\vec{\sigma}}\vec{E}\quad\text{, with }\ \vec{\vec{\sigma}}=i\varepsilon_0\omega\sum_s\alpha_s^2\begin{pmatrix}\dfrac{1}{1-\beta_s^2} & \dfrac{-i\beta_s}{1-\beta_s^2} & 0\\ \dfrac{i\beta_s}{1-\beta_s^2} & \dfrac{1}{1-\beta_s^2} & 0\\ 0 & 0 & 1\end{pmatrix}$$

where the sum is taken over particle species s. The dielectric tensor $\mathcal{E}$, with property:

$$\vec{k}\cdot(\vec{\vec{\mathcal{E}}}\cdot\vec{E})=0$$

is given by $\vec{\vec{\mathcal{E}}}=\vec{\vec{I}}-\vec{\vec{\sigma}}/i\varepsilon_0\omega$.

With the definitions $S=1-\displaystyle\sum_s\frac{\alpha_s^2}{1-\beta_s^2}$, $D=\displaystyle\sum_s\frac{\alpha_s^2\beta_s}{1-\beta_s^2}$, $P=1-\displaystyle\sum_s\alpha_s^2$

follows:

$$\vec{\vec{\mathcal{E}}}=\begin{pmatrix}S & -iD & 0\\ iD & S & 0\\ 0 & 0 & P\end{pmatrix}$$

The eigenvalues of this hermitian matrix are $R=S+D$, $L=S-D$, $\lambda_3=P$, with eigenvectors $\vec{e}_\mathrm{r}=\frac{1}{2}\sqrt{2}(1,i,0)$, $\vec{e}_\mathrm{l}=\frac{1}{2}\sqrt{2}(1,-i,0)$ and $\vec{e}_3=(0,0,1)$. $\vec{e}_\mathrm{r}$ is connected with a right rotating field for which $iE_x/E_y=1$ and $\vec{e}_\mathrm{l}$ is connected with a left rotating field for which $iE_x/E_y=-1$. When$k$ makes an angle θ with $\vec{B}$ one finds:

$$\tan^2(\theta)=\frac{P(n^2-R)(n^2-L)}{S(n^2-RL/S)(n^2-P)}$$

where n is the refractive index. From this the following solutions can be obtained:

A. $\theta=0$: transmission in the z-direction.

1. $P=0$: $E_x=E_y=0$. This describes a longitudinal linear polarized wave.
2. $n^2=L$: a left, circular polarized wave.
3. $n^2=R$: a right, circular polarized wave.

B. $\theta=\pi/2$: transmission ⊥ the B-field.

1. $n^2=P$: the ordinary mode: $E_x=E_y=0$. This is a transversal linear polarized wave.
2. $n^2=RL/S$: the extraordinary mode: $iE_x/E_y=-D/S$, an elliptical polarized wave.

Resonance frequencies are frequencies for which $n^2\rightarrow\infty$, so $v_\mathrm{f}=0$. For these holds: $\tan(\theta)=-P/S$. For $R\rightarrow\infty$ this gives the electron cyclotron resonance frequency $\omega=\Omega_\mathrm{e}$, for $L\rightarrow\infty$ the ion cyclotron resonance frequency $\omega=\Omega_\mathrm{i}$ and for $S=0$ holds for the extraordinary mode:

$$\alpha^2\left(1-\frac{m_\mathrm{i}}{m_\mathrm{e}}\frac{\Omega_\mathrm{i}^2}{\omega^2}\right)=\left(1-\frac{m_\mathrm{i}^2}{m_\mathrm{e}^2}\frac{\Omega_\mathrm{i}^2}{\omega^2}\right)\left(1-\frac{\Omega_\mathrm{i}^2}{\omega^2}\right)$$

Cut-off frequencies are frequencies for which $n^2=0$, so $v_\mathrm{f}\rightarrow\infty$. For these holds: $P=0$ or $R=0$ or $L=0$.

In the case that $\beta^2\gg1$ one finds Alfvén waves propagating parallel to the field lines. With the Alfvén velocity

$$v_\mathrm{A}=\frac{\Omega_\mathrm{e}\Omega_\mathrm{i}}{\omega_\mathrm{pe}^2+\omega_\mathrm{pi}^2}c^2$$

follows: $n=\sqrt{1+c/v_\mathrm{A}}$, and in case $v_\mathrm{A}\ll c$: $\omega=kv_\mathrm{A}$.

Chapter 12

Solid state physics

12.1 Crystal structure

A lattice is defined by the 3 translation vectors $\vec{a}_i$, so that the atomic composition looks the same from each point $\vec{r}$ and $\vec{r}\,' = \vec{r} + \vec{T}$, where $\vec{T}$ is a translation vector given by: $\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ with $u_i \in I\!N$. A lattice can be constructed from primitive cells. As primitive cell one can take a parallellepiped, with volume

$$V_{\rm cell} = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

Because a lattice has a periodical structure the physical properties who are connected with the lattice have the same periodicity (neglecting boundary effects):

$$n_{\rm e}(\vec{r} + \vec{T}\,) = n_{\rm e}(\vec{r}\,)\ .$$

This periodicity is excellent to use Fourier analysis: $n(\vec{r})$ is developed as:

$$n(\vec{r}) = \sum_G n_G \exp(i\vec{G} \cdot \vec{r}\,)$$

with

$$n_G = \frac{1}{V_{\rm cell}} \iiint\limits_{\rm cell} n(\vec{r}\,) \exp(-i\vec{G} \cdot \vec{r}\,) dV\ .$$

$\vec{G}$ is the *reciprocal lattice vector*. If $\vec{G}$ is written as $\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$ with $v_i \in I\!N$, follows for the vectors $\vec{b}_i$, cyclical:

$$\vec{b}_i = 2\pi \frac{\vec{a}_{i+1} \times \vec{a}_{i+2}}{\vec{a}_i \cdot (\vec{a}_{i+1} \times \vec{a}_{i+2})}\ .$$

The set of $\vec{G}$-vectors determines the Röntgen diffractions: a maximum in the reflected radiation occurs if: $\Delta\vec{k} = \vec{G}$ with $\Delta\vec{k} = \vec{k} - \vec{k}'$. So: $2\vec{k} \cdot \vec{G} = G^2$. From this follows for parallel lattice planes (Bragg reflection) that for the maxima holds: $2d\sin(\theta) = n\lambda$.

The Brillouin zone is defined as a Wigner-Seitz cell in the reciprocal lattice.

12.2 Crystal binding

A distinction can be made between 4 kinds of binding:

1. Van der Waals bond
2. Ion bond
3. Covalent or homopolar bond
4. Metalic bond.

At the ion binding of NaCl the energy per molecule is calculated by:

E = cohesive energy(NaCl) − ionization energy(Na) + electron affinity(Cl)

The interaction in a covalent bond depends on the relative spin orientations of the electrons forming the bond. The potential energy for two parallel spins is higher than the potential energy for two antiparallel spins. Further the potential energy for two parallel spins has sometimes no minimum. In that case binding is not possible.

12.3 Crystal vibrations

12.3.1 lattice with one kind of atoms

In this model for crystal vibrations, only nearest-neighbor interactions are taken into account. The force on atom s with mass M can then be written as:

$$F_s = M\frac{d^2u_s}{dt^2} = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

Assuming that all solutions have the same time-dependence $\exp(-i\omega t)$ this results in:

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

Further it is postulated that: $u_{s\pm1} = u\exp(isKa)\exp(\pm iKa)$.

This gives: $u_s = \exp(iKsa)$. Substituting of the later two equations in the first gives a system of linear equations, who have only a solution if their determinant is 0. This gives:

$$\omega^2 = \frac{4C}{M}\sin^2(\tfrac{1}{2}Ka)$$

Only vibrations with a wavelength within the first Brillouin Zone have a physical significance. This requires that $-\pi < Ka \leq \pi$.

The group velocity of these vibrations is given by:

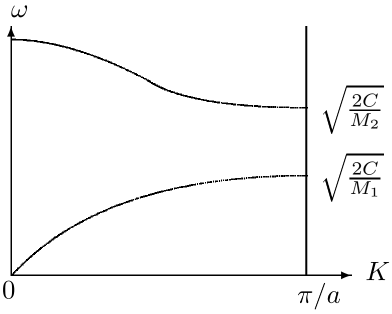
$$v_{\rm g} = \frac{d\omega}{dK} = \sqrt{\frac{Ca^2}{M}}\cos(\tfrac{1}{2}Ka)\ .$$

and is 0 on the edge of a Brillouin Zone. Here, there is a standing wave.

12.3.2 A lattice with two kinds of atoms

Now the solutions are:

$$\omega^2 = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2(Ka)}{M_1M_2}}$$



Connected with each value of ω are two values of K, as can be seen in the graph. The upper line describes the optical branch, the lower line the acoustical branch. In the optical branch, both kind of ions oscillate in opposite phases, in the acoustical branch they oscillate in the same phase. This results in a much larger induced dipole moment for optical oscillations, and also a stronger emission and absorption of radiation. Further each branch has 3 polarization directions, one longitudinal and two transversal.

12.3.3 Phonons

The quantummechanical excitation of a crystal vibration with an energy $\hbar\omega$ is called a *phonon*. Phonons can be viewed as quasi-particles: with collisions, they behave as particles with momentum $\hbar K$. Their total momentum is 0. When they collide, their momentum need not be conserved: for a normal process holds: $K_1 + K_2 = K_3$, for an umklapp process holds: $K_1 + K_2 = K_3 + G$. Because phonons have no spin they behave like bosons.

12.3.4 Thermal heat capacity

The total energy of the crystal vibrations can be calculated by multiplying each mode with its energy and sum over all branches K and polarizations P:

$$U=\sum_K\sum_P\hbar\omega\left\langle n_{k,p}\right\rangle=\sum_\lambda\int D_\lambda(\omega)\frac{\hbar\omega}{\exp(\hbar\omega/kT)-1}d\omega$$

for a given polarization λ. The thermal heat capacity is then:

$$C_{\rm rooster}=\frac{\partial U}{\partial T}=k\sum_\lambda\int D(\omega)\frac{(\hbar\omega/kT)^2\exp(\hbar\omega/kT)}{(\exp(\hbar\omega/kT)-1)^2}d\omega$$

The dispersion relation in one dimension is given by:

$$D(\omega)d\omega=\frac{L}{\pi}\frac{dK}{d\omega}d\omega=\frac{L}{\pi}\frac{d\omega}{v_{\rm g}}$$

In three dimensions one applies periodic boundary conditions on a cube with N^3 primitive cells and a volume L^3: $\exp(i(K_xx+K_yy+K_zz))\equiv\exp(i(K_x(x+L)+K_y(y+L)+K_z(z+L))$.

Because $\exp(2\pi i)=1$ this is only possible if:

$$K_x,K_y,K_z=0;\ \pm\frac{2\pi}{L};\ \pm\frac{4\pi}{L};\ \pm\frac{6\pi}{L};\ ...\pm\frac{2N\pi}{L}$$

So there is only one permitted value of $\vec{K}$ per volume $(2\pi/L)^3$ in K-space, or:

$$\left(\frac{L}{2\pi}\right)^3=\frac{V}{8\pi^3}$$

permitted $\vec{K}$-values per unit volume in $\vec{K}$-space, for each polarization and each branch. The total number of states with a wave vector $<K$ is:

$$N=\left(\frac{L}{2\pi}\right)^3\frac{4\pi K^3}{3}$$

for each polarization. The density of states for each polarization is, according to the Einstein model:

$$D(\omega)=\frac{dN}{d\omega}=\left(\frac{VK^2}{2\pi^2}\right)\frac{dK}{d\omega}=\frac{V}{8\pi^3}\iint\frac{dA_\omega}{v_{\rm g}}$$

The *Debye model* for thermal heat capacities is a low-temperature approximation which is valid till $\approx$ 50K. Here, only the acoustic phonons are taken into account (3 polarizations), and one assumes that $v=\omega K$, independent of the polarization. From this follows: $D(\omega)=V\omega^2/2\pi^2v^3$, where v is the speed of sound. This gives:

$$U=3\int D(\omega)\left\langle n\right\rangle\hbar\omega d\omega=\int\limits_0^{\omega_D}\frac{V\omega^2}{2\pi^2v^3}\frac{\hbar\omega}{\exp(\hbar\omega/kT)-1}d\omega=\frac{3Vk^2T^4}{2\pi^2v^3\hbar^3}\int\limits_0^{x_{\rm D}}\frac{x^3dx}{{\rm e}^x-1}\ .$$

Here, $x_{\rm D}=\hbar\omega_{\rm D}/kT=\theta_{\rm D}/T$. $\theta_{\rm D}$ is the *Debye temperature* and is defined by:

$$\theta_{\rm D}=\frac{\hbar v}{k}\left(\frac{6\pi^2N}{V}\right)^{1/3}$$

where N is the number of primitive cells. Because $x_{\rm D}\rightarrow\infty$ for $T\rightarrow0$ follows from this:

$$U=9NkT\left(\frac{T}{\theta_{\rm D}}\right)^3\int\limits_0^\infty\frac{x^3dx}{{\rm e}^x-1}=\frac{3\pi^4NkT^4}{5\theta_{\rm D}}\sim T^4\quad\text{and}\quad C_V=\frac{12\pi^4NkT^3}{5\theta_{\rm D}^3}\sim T^3$$

In the Einstein model for the thermal heat capacity one considers only phonons at one frequency, an approximation for optical phonons.

12.4 Magnetic field in the solid state

12.4.1 Dielectrics

The quantummechanical origin of diamagnetism is the Larmorprecession of the spin of the electron. Starting with a circular electron orbit in an atom with two electrons, there is a Coulomb force $F_{\rm c}$ and a magnetic force on each electron. If the magnetic part of the force is not strong enough to significant deform the orbit holds:

$$\omega^2 = \frac{F_{\rm c}(r)}{mr} \pm \frac{eB}{m}\omega = \omega_0^2 \pm \frac{eB}{m}(\omega_0+\delta) \Rightarrow \omega = \sqrt{\left(\omega_0 \pm \frac{eB}{2m}\right)^2 + \cdots} \approx \omega_0 \pm \frac{eB}{2m} = \omega_0 \pm \omega_{\rm L}$$

Here, $\omega_{\rm L}$ is the *Larmor frequency*. One electron is accelerated, the other decelerated. So there is a net circular current which results in a magnetic moment $\vec{\mu}$. The circular current is given by $I = -Ze\omega_{\rm L}/2\pi$, and $\langle\mu\rangle = IA = I\pi\left\langle\rho^2\right\rangle = \frac{2}{3}I\pi\left\langle r^2\right\rangle$. If N is the number of atoms in the crystal follows for the susceptibility, with $\vec{M} = \vec{\mu}N$:

$$\chi = \frac{\mu_0 M}{B} = -\frac{\mu_0 N Z e^2}{6m}\left\langle r^2\right\rangle$$

12.4.2 Paramagnetism

Starting with the splitting of energy levels in a weak magnetic field: $\Delta U_m - \vec{\mu}\cdot\vec{B} = m_J g\mu_{\rm B}B$, and with a distribution $f_m \sim \exp(-\Delta U_m/kT)$, one finds for the average magnetic moment $\langle\mu\rangle = \sum f_m\mu/\sum f_m$. After linearization, and because $\sum m_J = 0$, $\sum J = 2J+1$ and $\sum m_J^2 = \frac{2}{3}J(J+1)(J+\frac{1}{2})$ it follows that:

$$\chi_p = \frac{\mu_0 M}{B} = \frac{\mu_0 N\langle\mu\rangle}{B} = \frac{\mu_0 J(J+1)g^2\mu_{\rm B}^2 N}{3kT}$$

This is the *Curie law*, $\chi_p \sim 1/T$.

12.4.3 Ferromagnetism

A ferromagnet behaves like a paramagnet above a critical temperature $T_{\rm c}$. To describe ferromagnetism a field B_E parallel with M is postulated: $\vec{B}_E = \lambda\mu_0\vec{M}$. The treatment is further analogous with paramagnetism:

$$\mu_0 M = \chi_p(B_{\rm a} + B_E) = \chi_p(B_{\rm a} + \lambda\mu_0 M) = \mu_0\left(1 - \lambda\frac{C}{T}\right)M$$

From this follows for a ferromagnet: $\chi_F = \dfrac{\mu_0 M}{B_{\rm a}} = \dfrac{C}{T - T_{\rm c}}$ this is *Weiss-Curie's law.*

If B_E is estimated this way it results in values of about 1000 T. This is clearly unrealistic and suggests an other mechanism. A quantummechanical approach from Heisenberg postulates an interaction between two neighbor atoms: $U = -2J\vec{S}_i\cdot\vec{S}_j \equiv -\vec{\mu}\cdot\vec{B}_E$. J is an overlap integral given by: $J = 3kT_{\rm c}/2zS(S+1)$, with z the number of neighbors. A distinction between 2 cases can now be made:

1. $J > 0$: S_i and S_j become parallel: the material is a ferromagnet.
2. $J < 0$: S_i and S_j become antiparallel: the material is an antiferromagnet.

Heisenberg's theory predicts quantized spin waves: magnons. Starting with a model with only nearest neighbor interaction one can write:

$$U = -2J\vec{S}_p\cdot(\vec{S}_{p-1} + \vec{S}_{p+1}) \approx \vec{\mu}_p\cdot\vec{B}_p \quad \text{with} \quad \vec{B}_p = \frac{-2J}{g\mu_{\rm B}}(\vec{S}_{p-1} + \vec{S}_{p+1})$$

The equation of motion for the magnons becomes: $\displaystyle\frac{d\vec{S}}{dt}=\frac{2J}{\hbar}\vec{S}_p\times(\vec{S}_{p-1}+\vec{S}_{p+1})$

The treatment is further analogous with phonons: postulate traveling waves of the type $\vec{S}_p=\vec{u}\exp(i(pka-\omega t))$. This results in a system of linear equations with solution:

$$\hbar\omega=4JS(1-\cos(ka))$$

12.5 Free electron Fermi gas

12.5.1 Thermal heat capacity

The solution with period L of the one-dimensional Schrödinger equation is: $\psi_n(x)=A\sin(2\pi x/\lambda n)$ with $n\lambda_n=2L$. From this follows

$$E=\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

In a linear lattice the only important quantum numbers are n and m_s. The *Fermi level* is the uppermost filled level in the ground state, which has the *Fermi-energy* $E_{\rm F}$. If $n_{\rm F}$ is the quantum number of the Fermi level, it can be expressed as: $2n_{\rm F}=N$ so $E_{\rm F}=\hbar^2\pi^2N^2/8mL$. In 3 dimensions holds:

$$k_{\rm F}=\left(\frac{3\pi^2N}{V}\right)^{1/3}\quad\text{and}\quad E_{\rm F}=\frac{\hbar^2}{2m}\left(\frac{3\pi^2N}{V}\right)^{2/3}$$

The number of states with energy $\leq E$ is then: $\displaystyle N=\frac{V}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$.

and the density of states becomes: $\displaystyle D(E)=\frac{dN}{dE}=\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}=\frac{3N}{2E}$.

The heat capacity of the electrons is approximately 0.01 times the classical expected value $\frac{3}{2}Nk$. This is caused by the Pauli exclusion principle and the Fermi-Dirac distribution: only electrons within an energy range $\sim kT$ of the Fermi level are excited thermally. There is a fraction $\approx T/T_{\rm F}$ excited thermally. The internal energy then becomes:

$$U\approx NkT\frac{T}{T_{\rm F}}\quad\text{and}\quad C=\frac{\partial U}{\partial T}\approx Nk\frac{T}{T_{\rm F}}$$

A more accurate analysis gives: $C_{\rm electrons}=\frac{1}{2}\pi^2NkT/T_{\rm F}\sim T$. Together with the T^3 dependence of the thermal heat capacity of the phonons the total thermal heat capacity of metals is described by: $C=\gamma T+AT^3$.

12.5.2 Electric conductance

The equation of motion for the charge carriers is: $\vec{F}=md\vec{v}/dt=\hbar d\vec{k}/dt$. The variation of $\vec{k}$ is given by $\delta\vec{k}=\vec{k}(t)-\vec{k}(0)=-e\vec{E}t/\hbar$. If τ is the characteristic collision time of the electrons, $\delta\vec{k}$ remains stable if $t=\tau$. Then holds: $\langle\vec{v}\,\rangle=\mu\vec{E}$, with $\mu=e\tau/m$ the *mobility* of the electrons.

The current in a conductor is given by: $\vec{J}=nq\vec{v}=\sigma\vec{E}=\vec{E}/\rho=ne\mu\vec{E}$. Because for the collision time holds: $1/\tau=1/\tau_L+1/\tau_i$, where τ_L is the collision time with the lattice phonons and τ_i the collision time with the impurities, follows for the resistivity $\rho=\rho_L+\rho_i$, with $\lim\limits_{T\to0}\rho_L=0$.

12.5.3 The Hall-effect

If a magnetic field is applied $\perp$ at the direction of the current the charge carriers will be pushed aside by the Lorentz force. This results in a magnetic field $\perp$ the flow direction of the current. If $\vec{J}=J\vec{e}_x$ and $\vec{B}=B\vec{e}_z$ then $E_y/E_x=\mu B$. The Hall coefficient is defined by: $R_{\rm H}=E_y/J_xB$, and $R_{\rm H}=-1/ne$ if $J_x=ne\mu E_x$. The Hall voltage is given by: $V_{\rm H}=Bvb=IB/neh$ where b is the width of the material and h de height.

12.5.4 Thermal heat conductivity

With $\ell = v_F\tau$ the mean free path of the electrons follows from $\kappa = \frac{1}{3}C\,\langle v\rangle\,\ell$: $\kappa_{\rm electrons} = \pi^2 nk^2T\tau/3m$. From this follows for the *Wiedemann-Franz ratio*: $\kappa/\sigma = \frac{1}{3}(\pi k/e)^2T$.

12.6 Energy bands

In the *tight-bond* approximation it is assumed that $\psi = {\rm e}^{ikna}\phi(x-na)$. From this follows for the energy: $\langle E\rangle = \langle\psi|H|\psi\rangle = E_{\rm at} - \alpha - 2\beta\cos(ka)$. So this gives a cosine superimposed on the atomic energy, which can often be approximated with a harmonic oscillator. If it is assumed that the electron is nearly free one can postulate: $\psi = \exp(i\vec{k}\cdot\vec{r}\,)$. This is a traveling wave. This wave can be decomposed in two standing waves:

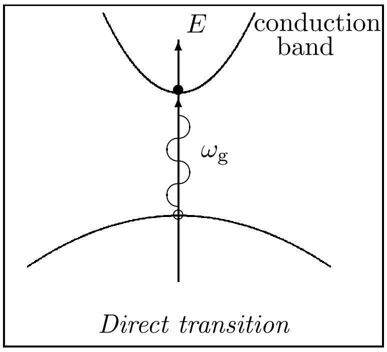
$$\begin{aligned}\psi(+) &= \exp(i\pi x/a) + \exp(-i\pi x/a) = 2\cos(\pi x/a)\\ \psi(-) &= \exp(i\pi x/a) - \exp(-i\pi x/a) = 2i\sin(\pi x/a)\end{aligned}$$

The probability density $|\psi(+)|^2$ is high near the atoms of the lattice and low between them. The probability density $|\psi(-)|^2$ is low near the atoms of the lattice and high between them. So the energy of $\psi(+)$ is also lower than the energy of $\psi)(-)$. Suppose that $U(x) = U\cos(2\pi x/a)$, than the bandgap is given by:

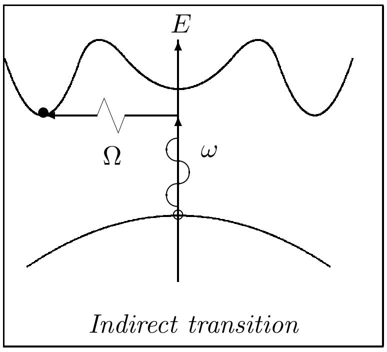
$$E_{\rm gap} = \int\limits_0^1 U(x)\left[|\psi(+)|^2 - |\psi(-)|^2\right]dx = U$$

12.7 Semiconductors

The band structures and the transitions between them of direct and indirect semiconductors are shown in the figures below. Here it is assumed that the momentum of the absorbed photon can be neglected. For an indirect semiconductor a transition from the valence to the conduction band is also possible if the energy of the absorbed photon is smaller than the band gap: then, also a phonon is absorbed.

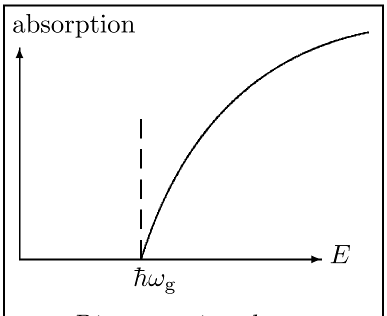


Direct transition

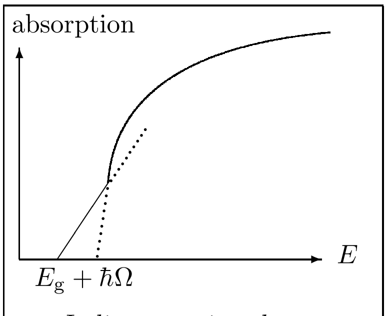


Indirect transition

This difference can also be observed in the absorption spectra:



Direct semiconductor



Indirect semiconductor

So indirect semiconductors, like Si and Ge, can not emit any light and are therefore not usable to fabricate lasers. When light is absorbed holds: $\vec{k}_{\rm h}=-\vec{k}_{\rm e}$, $E_{\rm h}(\vec{k}_{\rm h})=-E_{\rm e}(\vec{k}_{\rm e})$, $\vec{v}_{\rm h}=\vec{v}_{\rm e}$ and $m_{\rm h}=-m_{\rm e}^*$ if the conduction band and the valence band have the same structure.

Instead of the normal electron mass one has to use the *effective mass* within a lattice. It is defined by:

$$m^*=\frac{F}{a}=\frac{dp/dt}{dv_{\rm g}/dt}=\hbar\frac{dK}{dv_{\rm g}}=\hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}$$

with $E=\hbar\omega$ and $v_{\rm g}=d\omega/dk$ and $p=\hbar k$.

With the distribution function $f_{\rm e}(E)\approx\exp((\mu-E)/kT)$ for the electrons and $f_{\rm h}(E)=1-f_{\rm e}(E)$ for the holes the density of states is given by:

$$D(E)=\frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E-E_c}$$

with E_c the energy at the edge of the conductance band. From this follows for the concentrations of the holes p and the electrons n:

$$n=\int\limits_{E_c}^{\infty}D_{\rm e}(E)f_{\rm e}(E)dE=2\left(\frac{m^*kT}{2\pi\hbar^2}\right)^{3/2}\exp\left(\frac{\mu-E_{\rm c}}{kT}\right)$$

For the product np follows: $np=4\left(\dfrac{kT}{2\pi\hbar^2}\right)^3\sqrt{m_{\rm e}^*m_{\rm h}}\exp\left(-\dfrac{E_{\rm g}}{kT}\right)$

In an intrinsic (no impurities) semiconductor holds: $n_{\rm i}=p_{\rm i}$, in a $n-type$ holds: $n>p$ and in a $p-type$ holds: $n<p$.

An exciton is a bound electron-hole pair, rotating on each other as in positronium. The excitation energy of an exciton is smaller than the bandgap because the energy of an exciton is lower than the energy of a free electron and a free hole. This causes a peak in the absorption just before $E_{\rm g}$.

12.8 Superconductivity

12.8.1 Description

A superconductor is characterized by a zero resistivity if certain quantities are smaller than some critical values: $T<T_{\rm c}$, $I<I_{\rm c}$ and $H<H_{\rm c}$. The *BCS-model* predicts for the transition temperature $T_{\rm c}$:

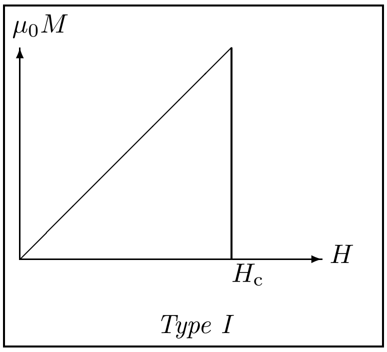
$$T_{\rm c}=1{,}14\Theta_{\rm D}\exp\left(\frac{-1}{UD(E_{\rm F})}\right)$$

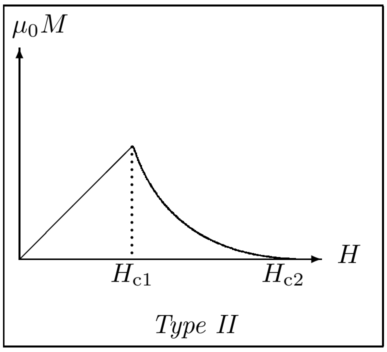
while experiments find for $H_{\rm c}$ in approximation:

$$H_{\rm c}(T)\approx H_{\rm c}(T_{\rm c})\left(1-\frac{T^2}{T_{\rm c}^2}\right)\ .$$

Within a superconductor the magnetic field is 0: the *Meissner effect*.

There are type I and type II superconductors. Because the Meissner effect implies that a superconductor is a perfect diamagnet holds in the superconducting state: $\vec{H}=\mu_0\vec{M}$. This holds for a type I superconductor, for a type II superconductor this only holds to a certain value $H_{\rm c1}$, for higher values of H the superconductor is in a *vortex state* to a value $H_{\rm c2}$, which can be 100 times $H_{\rm c1}$. If H becomes larger than $H_{\rm c2}$ the superconductor becomes a normal conductor. This is shown in the figures below.





The transition to a superconducting state is a second order thermodynamic state transition. This means that there is a twist in the $T-S$ diagram and a discontinuity in the C_X-T diagram.

12.8.2 The Josephson effect

For the Josephson effect one considers two superconductors, separated by an insulator. The electron wavefunction in one superconductor is ψ_1, in the other ψ_2. The Schrödinger equations in both superconductors is set equal:

$$i\hbar\frac{\partial\psi_1}{\partial t}=\hbar T\psi_2 \quad , \quad i\hbar\frac{\partial\psi_2}{\partial t}=\hbar T\psi_1$$

$\hbar T$ is the effect of the coupling of the electrons, or the transfer interaction through the insulator. The electron wavefunctions are written as $\psi_1=\sqrt{n_1}\exp(i\theta_1)$ and $\psi_2=\sqrt{n_2}\exp(i\theta_2)$. Because a Cooper pair exist of *two* electrons holds: $\psi\sim\sqrt{n}$. From this follows, if $n_1\approx n_2$:

$$\frac{\partial\theta_1}{\partial t}=\frac{\partial\theta_2}{\partial t} \quad\text{and}\quad \frac{\partial n_2}{\partial t}=-\frac{\partial n_1}{\partial t}$$

The Josephson effect results in a current density through the insulator depending on the phase difference as: $J=J_0\sin(\theta_2-\theta_1)=J_0\sin(\delta)$, where $J_0\sim T$. With an AC-voltage is across the junction the Schrödinger equations become:

$$i\hbar\frac{\partial\psi_1}{\partial t}=\hbar T\psi_2-eV\psi_1 \quad\text{and}\quad i\hbar\frac{\partial\psi_2}{\partial t}=\hbar T\psi_1+eV\psi_2$$

This gives: $J=J_0\sin\left(\theta_2-\theta_1-\dfrac{2eVt}{\hbar}\right)$.

So there is an oscillation with $\omega=2eV/\hbar$.

12.8.3 Fluxquantisation in a superconducting ring

For the current density in general holds: $\vec{J}=q\psi^*\vec{v}\psi=\dfrac{nq}{m}[\hbar\vec{\nabla}\theta-q\vec{A}\,]$

From the Meissner effect, $\vec{B}=0$ and $\vec{J}=0$, follows: $\hbar\vec{\nabla}\theta=q\vec{A}\Rightarrow\oint\vec{\nabla}\theta dl=\theta_2-\theta_1=2\pi s$ with $s\in I\!N$. Because: $\oint\vec{A}dl=\iint(\text{rot}\vec{A},\vec{n})d\sigma=\iint(\vec{B},\vec{n})d\sigma=\Psi$ follows: $\Psi=2\pi\hbar s/q$. The size of a flux quantum follows by setting $s=1$: $\Psi=2\pi\hbar/e=2,0678\cdot10^{-15}$ Tm^2.

12.8.4 Macroscopic quantum interference

From $\theta_2-\theta_1=2e\Psi/\hbar$ follows for two parallel junctions: $\delta_b-\delta_{\rm a}=\dfrac{2e\Psi}{\hbar}$, so

$J=J_{\rm a}+J_{\rm b}=2J_0\sin\left(\delta_0\cos\left(\dfrac{e\Psi}{\hbar}\right)\right)$ This gives maxima if $e\Psi/\hbar=s\pi$.

12.8.5 The London equation

A current density in a superconductor proportional with the vector potential $\vec{A}$ is postulated:

$$\vec{J}=\frac{-\vec{A}}{\mu_0\lambda_L^2}~~~\mbox{or}~~~\mbox{rot}\vec{J}=\frac{-\vec{B}}{\mu_0\lambda_L^2}$$

where $\lambda_L=\sqrt{\varepsilon_0 mc^2/nq^2}$. From this follows: $\nabla^2\vec{B}=\vec{B}/\lambda_L^2$.

The Meissner effect is the solution of this equation: $\vec{B}(x)=B_0\exp(-x/\lambda_L)$. Magnetic fields within a superconductor drop exponentially.

12.8.6 The BCS model

The BCS model can explain superconductivity from metals. (There is till now no explanation for high-$T_{\rm c}$ superconductance).
A new ground state where the electrons behave like independent fermions is postulated. Because the interaction with the lattice these pseudo-particles have a mutual attraction. This causes two electrons with opposite spin to combine to a *Cooper pair*. It can be proved that this ground state is perfect diamagnetic.

The infinite conductivity is more difficult to explain because a ring with a persisting current is not a real equilibrium: a state with zero current has a lower energy. Fluxquantization prevents transitions between these states. Fluxquantization is related with the existance of a coherent many-particle wavefunction. A flux quantum is the equivalent of about 10^4 electrons. So if the flux has to change with one flux quantum there has to occur a transition of many electrons, which is very improbable, or the system must go through intermediary states where the flux is not quantized so they have a higher energy. This is also very improbable.

Some useful mathematical relations are:

$$\int\limits_0^\infty\frac{xdx}{{\rm e}^{ax}+1}=\frac{\pi^2}{12a^2}~~,~~\int\limits_{-\infty}^\infty\frac{x^2dx}{({\rm e}^x+1)^2}=\frac{\pi^2}{3}~~,~~\int\limits_0^\infty\frac{x^3dx}{{\rm e}^x+1}=\frac{\pi^4}{15}$$

And, when $\sum\limits_{n=0}^\infty(-1)^n=\frac{1}{2}$ follows: $\int\limits_0^\infty\sin(px)dx=\int\limits_0^\infty\cos(px)dx=\frac{1}{p}$.

Chapter 13

Theory of groups

13.1 Introduction

13.1.1 Definition of a group

$\mathcal{G}$ is a group for the operation $\bullet$ if:

1. $\forall_{A,B\in\mathcal{G}} \Rightarrow A\bullet B\in\mathcal{G}$: $\mathcal{G}$ is *closed.*

2. $\forall_{A,B,C\in\mathcal{G}} \Rightarrow (A\bullet B)\bullet C = A\bullet(B\bullet C)$: $\mathcal{G}$ the *associative law.*

3. $\exists_{E\in\mathcal{G}}$ so that $\forall_{A\in\mathcal{G}} A\bullet E = E\bullet A = A$: $\mathcal{G}$ has a *unit element.*

4. $\forall_{A\in\mathcal{G}}\exists_{A^{-1}\in\mathcal{G}}$ z.d.d. $A\bullet A^{-1} = E$: Each element in $\mathcal{G}$ has an *inverse.*

If also holds:
5. $\forall_{A,B\in\mathcal{G}} \Rightarrow A\bullet B = B\bullet A$ the group is called *Abelian* or *commutative.*

13.1.2 The Cayley table

Each element arises only once in each row and column of the Cayley or multiplication table: because $EA_i = A_k^{-1}(A_kA_i) = A_i$ each A_i appears once. There are h positions in each row and column when there are h elements in the group so each elements appears only once.

13.1.3 Conjugated elements, subgroups and classes

B is *conjugate* with A if $\exists_{X\in\mathcal{G}}$ such that $B = XAX^{-1}$. Then A is also conjugate with B because $B = (X^{-1})A(X^{-1})^{-1}$.
If B and C are conjugate with A, B is also conjugate with C.

A *subgroup* is a subset of $\mathcal{G}$ which is also a group for the same operation.

A *conjugacy class* is the maximum collection of conjugated elements. Each group can be split up in conjugacy classes. Some theorems:

- All classes are completely disjoint.

- E is a class itself: for each other element in this class would hold: $A = XEX^{-1} = E$.

- E is the only class which is also a subgroup because all other classes have no unit element.

- In an Abelian group each element is a separate class.

The physical interpretation of classes: elements of a group are usually symmetry operations who map a symmetrical object on itself. Elements of one class are then the same kind of operations. The opposite need not to be true.

13.1.4 Isomorfism and homomorfism; representations

Two groups are *isomorphic* if they have the same multiplication table. The mapping from group $\mathcal{G}_1$ to $\mathcal{G}_2$, so that the multiplication table remains the same is a homomorphic mapping. It need not be isomorphic.

A *representation* is a homomorphic mapping of a group to a group of square matrices with the usual matrix multiplication as the combining operation. This is symbolized with Γ. The following holds:

$$\Gamma(E) = 1\!\!I \ \ , \ \ \Gamma(AB) = \Gamma(A)\Gamma(B) \ \ , \ \ \Gamma(A^{-1}) = [\Gamma(A)]^{-1}$$

For each group there are 3 possibilities for a representation:

1. A *faithful* representation: all matrices are different.
2. The representation $A \rightarrow \det(\Gamma(A))$.
3. The identical representation: $A \rightarrow 1$.

An *equivalent representation* is obtained by performing an unitary base transformation: $\Gamma'(A) = S^{-1}\Gamma(A)S$.

13.1.5 Reducible and irreducible representations

If *the same* unitary transformation can bring all matrices of a representation Γ in the same block structure the representation is called *reducible*:

$$\Gamma(A) = \begin{pmatrix} \Gamma^{(1)}(A) & 0 \\ 0 & \Gamma^{(2)}(A) \end{pmatrix}$$

This is written as: $\Gamma = \Gamma^{(1)} \oplus \Gamma^{(2)}$. If this is not possible the representation is called *irreducible.*

The number of irreducible representations equals the number of conjugacy classes.

13.2 The fundamental orthogonality theorem

13.2.1 Schur's lemma

Lemma: Each matrix who commutes with all matrices of an irreducible representation is a constant $\times 1\!\!I$, where $1\!\!I$ is the unit matrix. The opposite holds (of course) also.

Lemma If there exist a matrix M so that for two irreducible representations of group $\mathcal{G}$, $\gamma^{(1)}(A_i)$ and $\gamma^{(2)}(A_i)$, holds: $M\gamma^{(1)}(A_i) = \gamma^{(2)}(A_i)M$, the representations are equivalent, or $M = \underline{\underline{0}}$.

13.2.2 The fundamental orthogonality theorem

For a set of inequivalent, irreducible, unitary representations holds that, if h is the number of elements in the group and ℓ_i is the dimension of the $i^{\underline{\rm th}}$ representation:

$$\boxed{\sum_{R\in\mathcal{G}} \Gamma^{(i)*}_{\mu\nu}(R)\Gamma^{(j)}_{\alpha\beta}(R) = \frac{h}{\ell_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}}$$

13.2.3 Character

The *character* of a representation is given by the trace of the matrix and is therefore invariant for base transformations: $\boxed{\chi^{(j)}(R) = \mathrm{Tr}(\Gamma^{(j)}(R))}$

Also holds, with N_k the number of elements in a conjugacy class: $\boxed{\sum_k \chi^{(i)*}(C_k)\chi^{(j)}(C_k)N_k = h\delta_{ij}}$

Theorem: $\displaystyle\sum_{i=1}^{n} \ell_i^2 = h$

13.3 The relation with quantummechanics

13.3.1 Representations, energy levels and degeneracy

Consider a set of symmetry transformations $\vec{x}\,' = R\vec{x}$ who leave the Hamiltonian $\mathcal{H}$ invariant. These transformations are a group. An isomorfic operation on the wavefunction is given by: $P_R\psi(\vec{x}) = \psi(R^{-1}\vec{x})$. This is considered an *active rotation*. These operators commute with $\mathcal{H}$: $P_R\mathcal{H} = \mathcal{H}P_R$, and leave the volume element unchanged: $d(R\vec{x}) = d\vec{x}$.

P_R is the symmetry group of the physical system. It causes degeneracy: if ψ_n is a solution of $\mathcal{H}\psi_n = E_n\psi_n$ holds also: $\mathcal{H}(P_R\psi_n) = E_n(P_R\psi_n)$. A degeneracy who is not the result of a symmetry is called an *accidental degeneracy*.

Assume a ℓ_n-fold degeneracy at E_n: then choose an orthonormal set $\psi_\nu^{(n)}$, $\nu = 1, 2, \ldots, \ell_n$. The function $P_R\psi_\nu^{(n)}$ is in the same subspace: $P_R\psi_\nu^{(n)} = \displaystyle\sum_{\kappa=1}^{\ell_n} \psi_\kappa^{(n)}\Gamma_{\kappa\nu}^{(n)}(R)$

where $\Gamma^{(n)}$ is an *irreducible, unitary* representations of the symmetry group $\mathcal{G}$ of the system. Each n corresponds with an other energy level. One can purely mathematical derive irreducible representations of a symmetry group and label the energy levels with a quantum number this way. A fixed choice of $\Gamma^{(n)}(R)$ defines the base functions $\psi_\nu^{(n)}$. This way one can also label each separate base function with a quantum number.

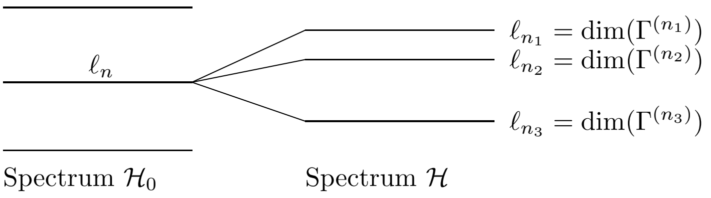
Particle in a periodical potential: the symmetry operation is a cyclic group: note the operator describing one translation over one unit as A. Then: $\mathcal{G} = \{A, A^2, A^3, \ldots, A^h = E\}$.
The group is Abelian so all irreducible representations are one-dimensional. For $0 \leq p \leq h-1$ follows:

$$\Gamma^{(p)}(A^n) = \mathrm{e}^{2\pi i p n/h}$$

If one defines: $k = -\dfrac{2\pi p}{ah}\left(\mathrm{mod}\dfrac{2\pi}{a}\right)$, so: $P_A\psi_p(x) = \psi_p(x-a) = \mathrm{e}^{2\pi i p/h}\psi_p(x)$, this gives *Bloch's theorem*: $\psi_k(x) = u_k(x)\mathrm{e}^{ikx}$, with $u_k(x \pm a) = u_k(x)$.

13.3.2 Breaking of degeneracy with a perturbation

Suppose the unperturbed system has Hamiltonian $\mathcal{H}_0$ and symmetry group $\mathcal{G}_0$. The perturbed system has $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$, and symmetry group $\mathcal{G} \subset \mathcal{G}_0$. If $\Gamma^{(n)}(R)$ is an irreducible representation of $\mathcal{G}_0$, it is also a representation of $\mathcal{G}$ but not all elements of $\Gamma^{(n)}$ in $\mathcal{G}_0$ are also in $\mathcal{G}$. The representation then usually becomes *reducible*: $\Gamma^{(n)} = \Gamma^{(n_1)} \oplus \Gamma^{(n_2)} \oplus \ldots$. The degeneracy is then (possibly partially) removed: see the figure below.



Theorem: The set of ℓ_n degenerated eigenfunctions $\psi_\nu^{(n)}$ with energy E_n is a basis for an ℓ_n-dimensional irreducible representation $\Gamma^{(n)}$ of the symmetry group.

13.3.3 The construction of a basefunction

Each function F in configuration space can be decomposed into *symmetry types*: $F = \displaystyle\sum_{j=1}^{n}\sum_{\kappa=1}^{\ell_j} f_\kappa^{(j)}$

The following operator extracts the symmetry types:

$$\left(\frac{\ell_j}{h}\sum_{R\in\mathcal{G}}\Gamma^{(j)*}_{\kappa\kappa}(R)P_R\right)F=f^{(j)}_\kappa$$

This is expressed as: $f^{(j)}_\kappa$ is the part of F that transforms according to the $\kappa^{\underline{\rm th}}$ row of $\Gamma^{(j)}$.

F can also be expressed in base functions φ: $F=\sum\limits_{aj\kappa}c_{aj\kappa}\varphi^{(aj)}_\kappa$. the functions $f^{(j)}_\kappa$ are in general not transformed into each other by elements of the group. However, this does happen if $c_{ja\kappa}=c_{ja}$.

Theorem: Two wavefunctions transforming according to non-equivalent unitary representations or according to different rows of an unitary irreducible representation are orthogonal:
$\langle\varphi^{(i)}_\kappa|\psi^{(j)}_\lambda\rangle\sim\delta_{ij}\delta_{\kappa\lambda}$, and $\langle\varphi^{(i)}_\kappa|\psi^{(i)}_\kappa\rangle$ is independent of κ.

13.3.4 The direct product of representations

Consider a physical system existing of two subsystems. The subspace $D^{(i)}$ of the system transforms according to $\Gamma^{(i)}$. Basefunctions are $\varphi^{(i)}_\kappa(\vec{x}_i)$, $1\leq\kappa\leq\ell_i$. Now form all $\ell_1\times\ell_2$ products $\varphi^{(1)}_\kappa(\vec{x}_1)\varphi^{(2)}_\lambda(\vec{x}_2)$. These define a space $D^{(1)}\otimes D^{(2)}$.

These product functions transform as:

$$P_R(\varphi^{(1)}_\kappa(\vec{x}_1)\varphi^{(2)}_\lambda(\vec{x}_2))=(P_R\varphi^{(1)}_\kappa(\vec{x}_1))(P_R\varphi^{(2)}_\lambda(\vec{x}_2))$$

In general the space $D^{(1)}\otimes D^{(2)}$ can be split up in a number of invariant subspaces:

$$\Gamma^{(1)}\otimes\Gamma^{(2)}=\sum_i n_i\Gamma^{(i)}$$

A useful tool for this reduction is that for the characters holds:

$$\chi^{(1)}(R)\chi^{(2)}(R)=\sum_i n_i\chi^{(i)}(R)$$

13.3.5 Clebsch-Gordan coefficients

At the reduction of the direct-product matrix w.r.t. the basis $\varphi^{(i)}_\kappa\varphi^{(j)}_\lambda$ one uses a new basis $\varphi^{(a\kappa)}_\mu$. These basefunctions lie in subspaces $D^{(ak)}$. The unitary base transformation is given by:

$$\varphi^{(ak)}_\mu=\sum_{\kappa\lambda}\varphi^{(i)}_\kappa\varphi^{(j)}_\lambda(i\kappa j\lambda|ak\mu)$$

and the inverse transformation by: $\varphi^{(i)}_\kappa\varphi^{(j)}_\lambda=\sum\limits_{ak\mu}\varphi^{(a\kappa)}_\mu(ak\mu|i\kappa j\lambda)$

The Clebsch-Gordan coefficients are dot products in essence: $(i\kappa j\lambda|ak\mu):=\langle\varphi^{(i)}_k\varphi^{(j)}_\lambda|\varphi^{(ak)}_\mu\rangle$

13.3.6 Symmetric transformations of operators, irreducible tensor operators

Observables (operators) transform as follows under symmetry transformations: $A'=P_RAP_R^{-1}$. If a set of operators $A^{(j)}_\kappa$ with $0\leq\kappa\leq\ell_j$ transform into each other under the transformations of $\mathcal{G}$ holds:

$$P_RA^{(j)}_\kappa P_R^{-1}=\sum_\nu A^{(j)}_\nu\Gamma^{(j)}_{\nu\kappa}(R)$$

If $\Gamma^{(j)}$ is irreducible they are called *irreducible tensor operators* $A^{(j)}$ with components $A^{(j)}_\kappa$.

Also an operator can be decomposed into symmetry types: $A=\sum\limits_{jk}a_k^{(j)}$, with:

$$a_\kappa^{(j)}=\left(\frac{\ell_j}{h}\sum_{R\in\mathcal{G}}\Gamma_{\kappa\kappa}^{(j)*}(R)\right)(P_RAP_R^{-1})$$

Theorem: Matrix elements H_{ij} of the operator $\mathcal{H}$ who is invariant under $\forall_{A\in\mathcal{G}}$, are 0 between states who transform according to non-equivalent irreducible unitary representations or according to different rows of such a representation. Further is $\langle\varphi_\kappa^{(i)}|\mathcal{H}|\psi_\kappa^{(i)}\rangle$ independent of κ. For $\mathcal{H}=1$ this becomes the previous theorem.

This is applied in quantum mechanics in *perturbation theory* and *variational calculus*. Here one tries to diagonalize $\mathcal{H}$. Solutions can be found within each category of functions $\varphi_\kappa^{(i)}$ with common i and κ: $\mathcal{H}$ is already diagonal in categories as a whole.
Perturbation calculus can be applied independent within each category. With variational calculus the try function can be chosen within a separate category because the exact eigenfunctions transform according to a row of an irreducible representation.

13.3.7 The Wigner-Eckart theorem

Theorem: The matrix element $\langle\varphi_\lambda^{(i)}|A_\kappa^{(j)}|\psi_\mu^{(k)}\rangle$ can only be $\neq 0$ if $\Gamma^{(j)}\otimes\Gamma^{(k)}=\ldots\oplus\Gamma^{(i)}\oplus\ldots$. If this is the case holds (if $\Gamma^{(i)}$ appears only once, otherwise one has to sum over a):

$$\boxed{\langle\varphi_\lambda^{(i)}|A_\kappa^{(j)}|\psi_\mu^{(k)}\rangle=(i\lambda|j\kappa k\mu)\langle\varphi^{(i)}\|A^{(j)}\|\psi^{(k)}\rangle}$$

This theorem can be used to determine selection rules: the probability on a dipole transition is given by ($\vec{\epsilon}$ is the direction of polarization of the radiation):

$$P_D=\frac{8\pi^2e^2f^3|r_{12}|^2}{3\hbar\varepsilon_0c^3}\quad\text{with}\quad r_{12}=\langle l_2m_2|\vec{\epsilon}\cdot\vec{r}\,|l_1m_1\rangle$$

Further it can be used to determine intensity ratios: if there is only one value of a the ratio of the matrix elements are the Clebsch-Gordan coefficients. For more a-values relations between the intensity ratios can be stated. However, the intensity ratios are also dependent on the occupation of the atomic energy levels.

13.4 Continuous groups

Continuous groups have $h=\infty$. However, not all groups with $h=\infty$ are continuous, e.g. the translation group of an spatially infinite periodic potential is not continuous but does have $h=\infty$.

13.4.1 The 3-dimensional translation group

For the translation of wavefunctions over a distance a holds: $P_a\psi(x)=\psi(x-a)$. Taylor development near x gives:

$$\psi(x-a)=\psi(x)-a\frac{d\psi(x)}{dx}+\frac{1}{2}a^2\frac{d^2\psi(x)}{dx^2}-+\ldots$$

Because the momentum operator in quantum mechanics is given by: $p_x=\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$, this can be written as:

$$\psi(x-a)=\mathrm{e}^{-iap_x/\hbar}\psi(x)$$

13.4.2 The 3-dimensional rotation group

This group is called SO(3) because a faithful representation can be constructed from orthogonal 3×3 matrices with a determinant of $+1$.

For an infinitesimal rotation around the x-axis holds:

$$\begin{array}{rcl}P_{\delta\theta_x}\psi(x,y,z) & \approx & \psi(x,y+z\delta\theta_x,z-y\delta\theta_x)\\ & = & \psi(x,y,z)+\left(z\delta\theta_x\frac{\partial}{\partial y}-y\delta\theta_x\frac{\partial}{\partial z}\right)\psi(x,y,z)\\ & = & \left(1-\frac{i\delta\theta_xL_x}{\hbar}\right)\psi(x,y,z)\end{array}$$

Because the angular momentum operator is given by: $L_x=\frac{\hbar}{i}\left(z\frac{\partial}{\partial y}-y\frac{\partial}{\partial z}\right)$.

So in an arbitrary direction holds: <u>Rotations:</u> $P_{\alpha,\vec{n}}=\exp(-i\alpha(\vec{n}\cdot\vec{J})/\hbar)$
<u>Translations:</u> $P_{a,\vec{n}}=\exp(-ia(\vec{n}\cdot\vec{p})/\hbar)$

J_x, J_y and J_z are called the *generators* of the 3-dim. rotation group, p_x, p_y and p_z are called the generators of the 3-dim. translation group.

The commutation rules for the generators can be derived from the properties of the group for multiplications: translations are interchangeable $\leftrightarrow p_xp_y-p_yp_x=0$.
Rotations are not generally interchangeable: consider a rotation around axis $\vec{n}$ in the xz-plane over an angle α. Then holds: $P_{\alpha,\vec{n}}=P_{-\theta,y}P_{\alpha,x}P_{\theta,y}$, so:

$$\mathrm{e}^{-i\alpha(\vec{n}\cdot\vec{J})/\hbar}=\mathrm{e}^{i\theta J_y/\hbar}\mathrm{e}^{-i\alpha J_x/\hbar}\mathrm{e}^{-i\theta J_y/\hbar}$$

If α and θ are very small and are developed till second order, and the corresponding terms are put equal with $\vec{n}\cdot\vec{J}=J_x\cos\theta+J_z\sin\theta$, follows from the $\alpha\theta$ term: $J_xJ_y-J_yJ_x=i\hbar J_z$.

13.4.3 Properties of continuous groups

The elements $R(p_1,...,p_n)$ depend continuous of parameters $p_1,...,p_n$. For the translation group this are e.g. an_x, an_y and an_z. It is demanded that the multiplication and inverse of an element R depend continuous of the de parameters of R.

The statement that each element arises only once in each row and column of the Cayley table holds also for continuous groups. The notion conjugacy class for continuous groups is defined equally as for discrete groups. The notion representation is fitted by demanding continuity: each matrix element depends continuous from $p_i(R)$.

Summation over all group elements is for continuous groups replaced with an integration. If $f(R)$ is a function defined on $\mathcal{G}$, e.g. $\Gamma_{\alpha\beta}(R)$, holds:

$$\int\limits_{\mathcal{G}}f(R)dR:=\int\limits_{p_1}\cdots\int\limits_{p_n}f(R(p_1,...,p_n))g(R(p_1,...,p_n))dp_1\cdots dp_n$$

Here, $g(R)$ is the *density function.*

Because of the properties of the Cayley table is demanded: $\int f(R)dR=\int f(SR)dR$. This fixes $g(R)$ except for a constant factor. Define new variables p' by: $SR(p_i)=R(p'_i)$. If one writes: $dV:=dp_1\cdots dp_n$ holds:

$$g(S)=g(E)\frac{dV}{dV'}$$

Here, $\frac{dV}{dV'}$ is the *Jacobian*: $\frac{dV}{dV'}=\det\left(\frac{\partial p_i}{\partial p'_j}\right)$, and $g(E)$ is constant.

For the translation group holds: $g(\vec{a}) = \text{constant} = g(\vec{0})$ because $g(a\vec{n}\ )d\vec{a}' = g(\vec{0})d\vec{a}$ and $d\vec{a}' = d\vec{a}$.

This leads to the fundamental orthogonality theorem:

$$\int_{\mathcal{G}} \Gamma_{\mu\nu}^{(i)*}(R)\Gamma_{\alpha\beta}^{(j)}(R)dR = \frac{1}{\ell_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}\int_{\mathcal{G}} dR$$

and for the characters holds:

$$\int_{\mathcal{G}} \chi^{(i)*}(R)\chi^{(j)}(R)dR = \delta_{ij}\int_{\mathcal{G}} dR$$

Compact groups are groups with a finite group volume: $\int_{\mathcal{G}} dR < \infty$.

13.5 The group SO(3)

One can take 2 parameters for the direction of the rotational axis and one for the angle of rotation φ. The parameter space is a collection points $\varphi\vec{n}$ within a sphere with radius π. The diametral points on this sphere are equivalent because $R_{\vec{n},\pi} = R_{\vec{n},-\pi}$.

An other way to define parameters is via *Eulers angle's*. If α, β and γ are the 3 Euler angles, defined as:

1. The spherical angles of axis 3 w.r.t. xyz are $\theta, \varphi := \beta, \alpha$. Now a rotation around axis 3 remains possible.
2. The spherical angles of the z-axis w.r.t. 123 are $\theta, \varphi := \beta, \pi - \gamma$.

then the rotation of a quantummechanical system is described with:
$\psi \to \mathrm{e}^{-i\alpha J_z\hbar}\mathrm{e}^{-i\beta J_y/\hbar}\mathrm{e}^{-i\gamma J_z/\hbar}\psi$. So $P_R = \mathrm{e}^{-i\varepsilon(\vec{n}\cdot\vec{J})/\hbar}$.

All irreducible representations of SO(3) can be constructed with the behaviour of the spherical harmonics $Y_{lm}(\theta,\varphi)$ with $-l \le m \le l$ and for a fixed l:

$$P_R Y_{lm}(\theta,\varphi) = \sum_{m'} Y_{lm'}(\theta,\varphi)D_{mm'}^{(l)}(R)$$

$D^{(l)}$ is an irreducible representation of dimension $2l+1$. The character of $D^{(l)}$ is given by:

$$\chi^{(l)}(\alpha) = \sum_{m=-l}^{l} \mathrm{e}^{im\alpha} = 1 + 2\sum_{k=0}^{l}\cos(k\alpha) = \frac{\sin([l+\frac{1}{2}]\alpha)}{\sin(\frac{1}{2}\alpha)}$$

In the used derivation α is the rotational angle around the z-axis. This expression holds for all rotations over an angle α because the classes of SO(3) are rotations around the same angle around an axis with an arbitrary orientation.

Via the the fundamental orthogonality theorem for characters one obtains the following expression for the density function (which is normalized so that $g(0) = 1$):

$$g(\alpha) = \frac{\sin^2(\frac{1}{2}\alpha)}{(\frac{1}{2}\alpha)^2}$$

With this result one can see that the given representations of SO(3) are the only ones: the character of another representation χ' would have to be $\perp$ the already found ones, so $\chi'(\alpha)\sin^2(\frac{1}{2}\alpha) = 0\forall\alpha \Rightarrow \chi'(\alpha) = 0\forall\alpha$. This is contradictionary because the dimension of the representation is given by $\chi'(0)$.

Because fermions have an half-odd integer spin the states ψ_{sm_s} with $s = \frac{1}{2}$ and $m_s = \pm\frac{1}{2}$ stretch a 2-dim. space which is invariant under rotations. A problem arises for rotations over 2π:

$$\psi_{\frac{1}{2}m_s} \to \mathrm{e}^{-2\pi i S_z/\hbar}\psi_{\frac{1}{2}m_s} = \mathrm{e}^{-2\pi i m_s}\psi_{\frac{1}{2}m_s} = -\psi_{\frac{1}{2}m_s}$$

However, in SO(3) holds: $R_{z,2\pi} = E$. So here holds $E \to \pm I\!\!I$. Because observable quantities can always be written as $\langle\phi|\psi\rangle$ or $\langle\phi|A|\psi\rangle$, and are bilinear in the states, they do not change sign if the states do. If only one state changes sign the observable quantities do change.

The existence of these half-odd integer representations is connected with the topological properties of SO(3): the group is two-fold coherent through the identification $R_0 = R_{2\pi} = E$.

13.6 Applications in quantum mechanics

13.6.1 Vectormodel for the addition of angular momentum

If two subsystems have angular momentum quantum numbers j_1 and j_2 the only possible values for the total angular momentum are $J = j_1 + j_2, j_1 + j_2 - 1, ..., |j_1 - j_2|$. This can be derived from group theory as follows: from $\chi^{(j_1)}(\alpha)\chi^{(j_2)}(\alpha) = \sum\limits_J n_J\chi^{(J)}(\alpha)$ follows:

$$D^{(j_1)} \otimes D^{(j_2)} = D^{(j_1+j_2)} \oplus D^{(j_1+j_2-1)} \oplus ... \oplus D^{(|j_1-j_2|)}$$

The states can be characterized with quantum numbers in two ways: with j_1, m_1, j_2, m_2 and with j_1, j_2, J, M. The Clebsch-Gordan coefficients, for SO(3) called the *Wigner coefficients* can be chosen real, so:

$$\begin{array}{lll}\psi_{j_1j_2JM} & = & \sum\limits_{m_1m_2}\psi_{j_1m_1j_2m_2}(j_1m_1j_2m_2|JM)\\ \psi_{j_1m_1j_2m_2} & = & \sum\limits_{JM}\psi_{j_1j_2JM}(j_1m_1j_2m_2|JM)\end{array}$$

13.6.2 Irreducible tensoroperators, matrixelements and selection rules

Some examples of the behaviour of operators under SO3)

1. Suppose $j = 0$: this gives the identical representation with $\ell_j = 1$. This state is described with a scalar operator. Because $P_RA_0^{(0)}P_R^{-1} = A_0^{(0)}$ this operator is invariant, e.g. the Hamiltonian of a free atom. Then holds: $\langle J'M'|\mathcal{H}|JM\rangle \sim \delta_{MM'}\delta_{JJ'}$.

2. A vector operator: $\vec{A} = (A_x, A_y, A_z)$. The cartesian components of a vector operator transform equally as the cartesian components of $\vec{r}$ by definition. So for rotations around the z-axis holds:

   $$D(R_{\alpha,z}) = \left(\begin{array}{ccc}\cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1\end{array}\right)$$

   The transformed operator has the same matrix elements w.r.t. $P_R\psi$ and $P_R\phi$: $\left\langle P_R\psi|P_RA_xP_R^{-1}|P_R\phi\right\rangle = \langle\psi|A_x|\phi\rangle$. $\chi(R_{\alpha,z}) = 1 + 2\cos(\alpha)$. According to the equation for characters this means one can choose base operators who transform like $Y_{1m}(\theta, \varphi)$. This turn out to be the spherical components:

   $$A_{+1}^{(1)} = -\frac{1}{\sqrt{2}}(A_x + iA_y),\quad A_0^{(1)} = A_z,\quad A_{-1}^{(1)} = \frac{1}{\sqrt{2}}(A_x - iA_y)$$

3. A cartesian tensor of rank 2: T_{ij} is a quantity which transforms under rotations like U_iV_j, where $\vec{U}$ and $\vec{V}$ are vectors. So T_{ij} transforms like $P_RT_{ij}P_R^{-1} = \sum\limits_{kl}T_{kl}D_{ki}(R)D_{lj}(R)$, so like $D^{(1)} \otimes D^{(1)} = D^{(2)} \oplus D^{(1)} \oplus D^{(0)}$. The 9 components can be split in 3 invariant subspaces with dimension 1 ($D^{(0)}$), 3 ($D^{(1)}$) and 5 ($D^{(2)}$). The new base operators are:

   I. $\text{Tr}(\underline{\underline{T}}) = T_{xx} + T_{yy} + T_{zz}$. This transforms as the scalar $\vec{U} \cdot \vec{V}$, so as $D^{(0)}$.

   II. The 3 antisymmetric components $A_z = \frac{1}{2}(T_{xy} - T_{yx})$, etc. These transform as the vector $\vec{U} \times \vec{V}$, so as $D^{(1)}$.

   III. The 5 independent components of the traceless, symmetric tensor $\underline{\underline{S}}$: $S_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}\delta_{ij}\text{Tr}(\underline{\underline{T}})$. These transform as $D^{(2)}$.

Selection rules for dipole transitions

Dipole operators transform as $D^{(1)}$: for an electric dipole transfer is the operator $e\vec{r}$, for a magnetic $\frac{e}{2m}(\vec{L}+2\vec{S})$.

From the Wigner-Eckart theorem follows: $\langle J'M'|A_\kappa^{(1)}|JM\rangle=0$ except $D^{(J')}$ is a part of $D^{(1)}\otimes D^{(J)}=D^{(J+1)}\oplus D^{(J)}\oplus D^{(|J-1|)}$. This means that $J'\in\{J+1,J,|J-1|\}$: $J'=J$ or $J'=J\pm1$, except $J'=J=0$.

Landé-equation for the anomalous Zeeman splitting

According to Landé's model the interaction between a magnetic moment with an external magnetic field is determined by the projection of $\vec{M}$ on $\vec{J}$ because $\vec{L}$ and $\vec{S}$ precede fast on $\vec{J}$. This can also be understood from the Wigner-Eckart theorem: from this follows that the matrix elements from all vector operators show a certain proportionality. For an arbitrary operator $\vec{A}$ follows:

$$\langle\alpha jm'|\vec{A}|\alpha jm\rangle=\frac{\langle\alpha jm|\vec{A}\cdot\vec{J}\,|\alpha jm\rangle}{j(j+1)\hbar^2}\,\langle\alpha jm'|\vec{J}\,|\alpha jm\rangle$$

13.7 Applications in particle physics

The physics of a system does not change after performing a transformation $\psi'=\mathrm{e}^{i\delta}\psi$ where δ is a constant. This is a *global gauge transformation*: the phase of the wavefunction changes everywhere with the same amount.

There exist some freedom in the choice of the potentials $\vec{A}$ and ϕ at the same $\vec{E}$ and $\vec{B}$: *gauge transformations* of the potentials do not change $\vec{E}$ and $\vec{B}$ (See chapter 2 and 10). The solution ψ' of the Schrödinger equation with the transformed potentials is: $\psi'=\mathrm{e}^{-iqf(\vec{r},t)}\psi$.

This is a *local gauge transformation*: the phase of the wavefunction changes different at each position. The physics of the system does not change if $\vec{A}$ and ϕ are also transformed. This is now stated as guide principle: *the "right of existence" of the electromagnetic field is to allow local gauge invariance.*

The gauge transformations of the EM-field form a group: U(1), unitary 1×1-matrices. The split-off of charge in the exponent is essential: it allows one gauge field for all charged particles, independent of their charge.

This concept is generalized: particles have a "special charge" Q. The group elements now are $P_R=\exp(-iQ\Theta)$.

Other force fields than the electromagnetic field can also be understood this way. The weak interaction together with the electromagnetic interaction can be described with a force field that transforms according to U(1)⊗SU(2), and consists of the photon and three intermediar vector bosons. The color force is described by SU(3), and has a gauge field that exist of 8 types of gluons.

In general the group elements are given by $P_R=\exp(-i\vec{T}\cdot\vec{\Theta})$, where Θ_n are real constants and T_n operators (generators), like Q. The commutation rules are given by $[T_i,T_j]=i\sum\limits_k c_{ijk}T_k$. The c_{ijk} are the *structure constants* of the group. For SO(3) these constants are $c_{ijk}=\varepsilon_{ijk}$, here ε_{ijk} is the complete antisymmetric tensor with $\varepsilon_{123}=+1$.

These constants can be found with the help of group product elements: because $\mathcal{G}$ is closed holds: $\mathrm{e}^{i\vec{\Theta}\cdot\vec{T}}\mathrm{e}^{i\vec{\Theta}'\cdot\vec{T}}\mathrm{e}^{-i\vec{\Theta}\cdot\vec{T}}\mathrm{e}^{-i\vec{\Theta}'\cdot\vec{T}}=\mathrm{e}^{-i\vec{\Theta}''\cdot\vec{T}}$. Taylor development and setting equal $\Theta^n\Theta'^m$-terms results in the commutation rules.

The group SU(2) has 3 free parameters: because it is unitary there are 4 real conditions on 4 complex parameters, and the determinant has to be +1, remaining 3 free parameters.

Each unitary matrix U can be written as: $U=\mathrm{e}^{-iH}$. Here, H is a Hermitian matrix. Further holds always: $\det(U)=\mathrm{e}^{-i\mathrm{Tr}(H)}$.
For each matrix of SU(2) holds that Tr(H)=0. Each Hermitian, traceless 2×2 matrix can be written

as a linear combination of the 3 *Pauli-matrices* σ_i. So these matrices are a choice for the operators of SU(2). One can write: SU(2)=$\{\exp(-\frac{1}{2}i\vec{\sigma}\cdot\vec{\Theta})\}$.

Abstractly, one can consider an isomorphic group where only the commutation rules are considered known about the operators T_i: $[T_1,T_2]=iT_3$, etc.

In elementary particle physics the T_i can be interpreted e.g. as the *isospin* operators. Elementary particles can be classified in isospin-multiplets, this are the irreducible representations of SU(2). The classification is:

1. The isospin-singlet ≡ the identical representation: $\mathrm{e}^{-i\vec{T}\cdot\vec{\Theta}}=1\Rightarrow T_i=0$
2. The isospin-doublet ≡ the faithful representation of SU(2) on 2×2 matrices.

The group SU(3) has 8 free parameters. (The group SU(N) has N^2-1 free parameters). The Hermitian, traceless operators are 3 SU(2)-subgroups in the $\vec{e}_1\vec{e}_2$, $\vec{e}_1\vec{e}_3$ and the $\vec{e}_2\vec{e}_3$ plane. This gives 9 matrices, who are not all 9 linear independent. By taking a linear combination one gets 8 matrices.

In the Lagrange density for the color force one has to substitute $\displaystyle\frac{\partial}{\partial x}\rightarrow\frac{D}{Dx}:=\frac{\partial}{\partial x}-\sum_{i=1}^{8}T_iA_x^i$

The terms of 3rd and 4th power in A show that the color field interacts with itself.

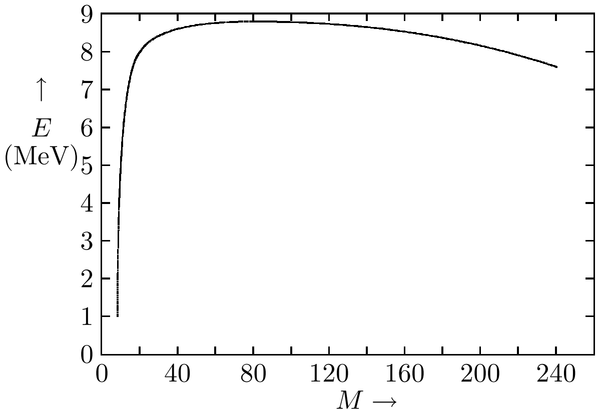
Chapter 14

Nuclear physics

14.1 Nuclear forces

The mass of a nucleus is given by:

$$M_{\text{nucl}} = Zm_{\text{p}} + Nm_{\text{n}} - E_{\text{bind}}/c^2$$



The binding energy per nucleon is given in the figure at the right. The top is at $^{56}_{26}$Fe, the most stable nucleus. With the constants

$$\begin{array}{lcrl} a_1 & = & 15{,}760 & \text{MeV} \\ a_2 & = & 17{,}810 & \text{MeV} \\ a_3 & = & 0{,}711 & \text{MeV} \\ a_4 & = & 23{,}702 & \text{MeV} \\ a_5 & = & 34{,}000 & \text{MeV} \end{array}$$

is in the *droplet* or *collective model* of the nucleus the binding energy E_{bind} given by:

$$\frac{E_{\text{bind}}}{c^2} = a_1 A - a_2 A^{2/3} - a_3 \frac{Z(Z-1)}{A^{1/3}} - a_4 \frac{(N-Z)^2}{A} + \epsilon a_5 A^{-3/4}$$

These terms arise from:

1. a_1: Binding energy of the strong nuclear force, approximately $\sim A$.
2. a_2: Surface correction: the nucleons near the surface are less bound.
3. a_3: Coulomb repulsion between the protons.
4. a_4: Asymmetry term: a surplus of protons or neutrons has a lower binding energy.
5. a_5: Pair off effect: nuclei with an even number of protons or neutrons are more stable because groups of two protons or neutrons have a lower energy. The following holds:

   $\underline{Z \text{ even}, N \text{ even:}}$ $\epsilon = +1$, $\underline{Z \text{ odd}, N \text{ odd:}}$ $\epsilon = -1$.
   $\underline{Z \text{ even}, N \text{ odd:}}$ $\epsilon = 0$, $\underline{Z \text{ odd}, N \text{ even:}}$ $\epsilon = 0$.

The Yukawa potential can be derived if the nuclear force can, in first approximation, be considered an exchange of virtual pions:

$$U(r) = -\frac{W_0 r_0}{r} \exp\left(-\frac{r}{r_0}\right)$$

With $\Delta E \cdot \Delta t \approx \hbar$, $r_0 = c\Delta t$ and $E_\gamma = m_0 c^2$ holds: $r_0 = \hbar/m_0 c$.

In the shell model of the nucleus one assumes that a nucleon moves in an average field of other nucleons. Further, there is a contribution of the spin-orbit coupling $\sim \vec{L} \cdot \vec{S}$: $\Delta V_{ls} = \frac{1}{2}(2l+1)\hbar\omega$. So each level (n,l) niveau is split in two, with $j = l \pm \frac{1}{2}$, where the state with $j = l + \frac{1}{2}$ has the lowest energy. This is just the opposite for electrons, which is an indication that the $L - S$ interaction is not electromagnetical. The energy of a 3-dimensional harmonic oscillator is $E = (N + \frac{3}{2})\hbar\omega$. $N = n_x + n_y + n_z = 2(n-1) + l$ where $n \geq 1$ is the main oscillator number. Because $-l \leq m \leq l$

and $m_s = \pm\frac{1}{2}\hbar$ there are $2(2l+1)$ substates who exist independent for protons and neutrons. This gives rise to the so called *magical numbers*: nuclei where each state in the outermost level are filled are especially stable. This is the case if N or $Z \in \{2, 8, 20, 28, 50, 82, 126\}$.

14.2 The shape of the nucleus

An nucleus is in first approximation spherical with a radius of $R = R_0 A^{1/3}$. Here, $R_0 \approx 1,4 \cdot 10^{-15}$ m, constant for all nuclei. If the nuclear radius is measured with the charge distribution one obtains $R_0 \approx 1,2 \cdot 10^{-15}$ m. The shape of oscillating nuclei can be described with spherical harmonics:

$$R = R_0 \left[1 + \sum_{lm} a_{lm} Y_l^m(\theta, \varphi) \right]$$

$l = 0$ gives rise to monopole vibrations, density vibrations, who can be applied in the theory of neutron stars. $l = 1$ gives dipole vibrations, $l = 2$ quadrupole, with $a_{2,0} = \beta \cos\gamma$ and $a_{2,\pm2} = \frac{1}{2}\sqrt{2}\beta \sin\gamma$ where β is the deformation factor and γ the shape parameter. The multipole moment is given by $\mu_l = Zer^l Y_l^m(\theta, \varphi)$. The parity of the electric moment is $\Pi_E = (-1)^l$, of the magnetic moment $\Pi_M = (-1)^{l+1}$.

There are 2 contributions to the magnetic moment: $\vec{M}_L = \dfrac{e}{2m_{\rm p}}\vec{L}$ and $\vec{M}_S = g_S \dfrac{e}{2m_{\rm p}}\vec{S}$.

where g_S is the *spin-gyromagnetic ratio*. For protons holds $g_S = 5,5855$ and for neutrons $g_S = -3,8263$. The z-components of the magnetic moment are given by $M_{L,z} = \mu_{\rm N} m_l$ and $M_{S,z} = g_S \mu_{\rm N} m_S$. The resulting magnetic moment is related to the nuclear spin I according to $\vec{M} = g_I(e/2m_{\rm p})\vec{I}$. The z-component is then $M_z = \mu_{\rm N} g_I m_I$.

14.3 Radioactive decay

The number of nuclei decaying is proportional with the number of nuclei: $\dot{N} = -\lambda N$. This gives for the number of nuclei N: $N(t) = N_0 \exp(-\lambda t)$. The *half life time* follows from $\tau_{\frac{1}{2}}\lambda = \ln(2)$. The average life time of a nucleus is $\tau = 1/\lambda$. The probability that N nuclei decay within a time interval is governed by a Poisson distribution:

$$P(N)dt = N_0 \frac{\lambda^N {\rm e}^{-\lambda}}{N!} dt$$

If a nucleus can decay to more final states holds: $\lambda = \sum \lambda_i$. So the fraction decaying to state i is $\lambda_i / \sum \lambda_i$. There are 5 types of natural radioactive decay:

1. α-decay: the nucleus emits a He^{2+} nucleus. Because nucleons tend to order themselves in groups of 2p+2n this can be considered as a tunneling of a He^{2+} nucleus through a potential barrier. The tunnel probability P is

$$P = \frac{\text{amplitude incoming}}{\text{amplitude outgoing}} = {\rm e}^{-2G} \quad \text{with} \quad G = \frac{1}{\hbar}\sqrt{2m \int [V(r) - E]dr}$$

   G is called the *Gamow factor*.

2. β-decay. Here a proton changes into a neutron or vice versa:
   $\mathrm{p}^+ \rightarrow \mathrm{n}^0 + \mathrm{W}^+ \rightarrow \mathrm{n}^0 + \mathrm{e}^+ + \nu_{\rm e}$, and $\mathrm{n}^0 \rightarrow \mathrm{p}^+ + \mathrm{W}^- \rightarrow \mathrm{p}^+ + \mathrm{e}^- + \overline{\nu}_{\rm e}$.

3. Electron capture: here, a proton in the nucleus captures an electron (usually from the K-shell).

4. Spontaneous fission: a nucleus breaks apart.

5. γ-decay: here the nucleus emits a high-energetic photon. The decay constant is given by

$$\lambda = \frac{P(l)}{\hbar\omega} \sim \left(\frac{E_\gamma R}{\hbar c}\right)^{2l} \sim 10^{-4l}$$

where l is the quantum number for the angular momentum and P the radiated power. Usually the decay constant of electric multipole moments is larger than the one of magnetic multipole moments. The energy of the photon is $E_\gamma = E_i - E_f - T_{\rm R}$, with $T_{\rm R} = E_\gamma^2/2mc^2$ the recoil energy, which can usually be neglected. The parity of the emitted radiation is $\Pi^l = \Pi^i \cdot \Pi^f$. With I the quantum number of angular momentum of the nucleus, $L = \hbar\sqrt{I(I+1)}$, holds the following selection rule: $|\vec{I}_i - \vec{I}_f| \leq \Delta l \leq |\vec{I}_i + \vec{I}_f|$.

14.4 Scattering and nuclear reactions

14.4.1 Kinetic model

If a beam with intensity I hits a target with density n and length x (Rutherford scattering) the number of scatterings R per unit of time is equal to $R = Inx\sigma$. From this follows that the intensity of the beam decreases as $-dI = In\sigma dx$. This results in $I = I_0{\rm e}^{-n\sigma x} = I_0{\rm e}^{-\mu x}$.

Because $dR = R(\theta,\varphi)d\Omega/4\pi = Inxd\sigma$ follows: $\displaystyle\frac{d\sigma}{d\Omega} = \frac{R(\theta,\varphi)}{4\pi nxI}$

If N particles are scattered in a material with density n holds: $\displaystyle\frac{\Delta N}{N} = n\frac{d\sigma}{d\Omega}\Delta\Omega\Delta x$

For Coulomb collisions holds: $\displaystyle\left.\frac{d\sigma}{d\Omega}\right|_{\rm C} = \frac{Z_1Z_2e^2}{8\pi\varepsilon_0\mu v_0^2}\frac{1}{\sin^4(\frac{1}{2}\theta)}$

14.4.2 Quantummechanical model for n-p scattering

The initial state is a beam of neutrons moving among the z-axis with wavefunction $\psi_{\rm init} = {\rm e}^{ikz}$ and current density $J_{\rm init} = v|\psi_{\rm init}|^2 = v$. At large distastances from the scattering point they have approximately a spherical wavefunction $\psi_{\rm scat} = f(\theta){\rm e}^{ikr}/r$ where $f(\theta)$ is the *scattering amplitude.* The total wavefunction is then given by

$$\psi = \psi_{\rm in} + \psi_{\rm scat} = {\rm e}^{ikz} + f(\theta)\frac{{\rm e}^{ikr}}{r}$$

The particle flux of the scattered particles is $v|\psi_{\rm scat}|^2 = v|f(\theta)|^2 d\Omega$. From this follows that $\sigma(\theta) = |f(\theta)|^2$. The wavefunction of the incoming particles can be expressed in a sum of angular momentum wavefunctions:

$$\psi_{\rm init} = {\rm e}^{ikz} = \sum_l \psi_l$$

The impactparameter is related to the angular momentum with $L = bp = b\hbar k$, so $bk \approx l$. For very low energy only particles with $l = 0$ are scattered, so

$$\psi = \psi_0' + \sum_{l>0}\psi_l \quad \text{and} \quad \psi_0 = \frac{\sin(kr)}{kr}$$

If the potential is approximately rectangular holds: $\displaystyle\psi_0' = C\frac{\sin(kr+\delta_0)}{kr}$

The cross section is then $\displaystyle\sigma(\theta) = \frac{\sin^2(\delta_0)}{k^2}$ so $\displaystyle\sigma = \int\sigma(\theta)d\Omega = \frac{4\pi\sin^2(\delta_0)}{k^2}$

For very low energies holds: $\displaystyle\sin^2(\delta_0) = \frac{\hbar^2k^2/2m}{W_0+W}$

with W_0 the depth of the potential well. For higher energies holds: $\displaystyle\sigma = \frac{4\pi}{k^2}\sum_l \sin^2(\delta_l)$

14.4.3 Conservation of energy and momentum in nuclear reactions

If a particle P_1 collides with a particle P_2 which is in rest w.r.t. the laboratory system and other particles are created, so

$$P_1 + P_2 \rightarrow \sum_{k>2} P_k$$

the total energy Q gained or required is given by $Q = (m_1 + m_2 - \sum\limits_{k>2} m_k)c^2$.

The minimal required kinetic energy T of P_1 in the laboratory system to initialize the reaction is

$$T = -Q\frac{m_1 + m_2 + \sum m_k}{2m_2}$$

If $Q < 0$ there is a threshold energy.

14.5 Radiation dosimetry

Radiometric quantities determine the strength of the radiation source(es). *Dosimetric quantities* are related to the energy transfer from radiation to matter. Parameters describing a relation between those are called *interaction parameters*. The intensity of a beam of particles in matter decreases according to $I(s) = I_0\exp(-\mu s)$. The deceleration of a *heavy* particle is described with the *Bethe-Bloch equation*:

$$\frac{dE}{ds} \sim \frac{q^2}{v^2}$$

The *fluention* is given by $\Phi = dN/dA$. The *flux* is given by $\phi = d\Phi/dt$. The energy loss is defined by $\Psi = dW/dA$, and the energy flux density $\psi = d\Psi/dt$. The *absorption coefficient* is given by $\mu = (dN/N)/dx$. The *mass absorption coefficient* is given by μ/ϱ.

The *radiation dose* X is amount of charge produced by the radiation per unit of mass, with unit C/kg. An old unit is the Röntgen: 1Ro= $2,58 \cdot 10^{-4}$ C/kg. With the energy-absorption coefficient μ_E follows:

$$X = \frac{dQ}{dm} = \frac{e\mu_E}{W\varrho}\Psi$$

where W is the energy required to free an elementary charge.

The *absorbed dose* D is given by $D = dE_{\rm abs}/dm$, with unit Gy=J/kg. An old unit is the rad: 1 rad=0,01 Gy. The *dose tempo* is defined as $\dot{D}$. It can be derived that

$$D = \frac{\mu_E}{\varrho}\Psi$$

The *Kerma* K is the amount of kinetic energy of secundary produced particles which is produced per mass unit of the radiated object.

The *equivalent dose* H is an weight average of the absorbed dose per type of radiation, where for each type radiation the effects on biological material is used for the weigh factor. These weigh factors are called the quality factors. Their unit is Sv. $H = QD$. If the absorption is not equally distributed also weigh factors w per organ needs to be used: $H = \sum w_k H_k$. For some types of radiation holds:

Radiation type	Q
Röntgen, gamma radiation	1
β, electrons, mesons	1
Thermic neutrons	3 to 5
Fast neutrons	10 to 20
protons	10
α, fission products	20

Chapter 15

Quantum field theory & Particle physics

15.1 Creation and annihilation operators

A state with more particles can be described with a collection occupation numbers $|n_1 n_2 n_3 \cdots\rangle$. So the vacuum state is given by $|000\cdots\rangle$. This is a complete description because the particles are indistinguishable. The states are orthonormal:

$$\langle n_1 n_2 n_3 \cdots | n_1' n_2' n_3' \cdots\rangle = \prod_{i=1}^{\infty} \delta_{n_i n_i'}$$

The time-dependent state vector is given by

$$\Psi(t) = \sum_{n_1 n_2 \cdots} c_{n_1 n_2 \cdots}(t) | n_1 n_2 \cdots\rangle$$

The coefficients c can be interpreted as follows: $|c_{n_1 n_2 \cdots}|^2$ is the probability to find n_1 particles with momentum $\vec{k}_1$, n_2 particles with momentum $\vec{k}_2$, etc., and $\langle\Psi(t)|\Psi(t)\rangle = \sum |c_{n_i}(t)|^2 = 1$. The development of the states in time is described by the Schrödinger equation

$$i\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

where $H = H_0 + H_{\rm int}$. H_0 is the Hamiltonian for free particles and keeps $|c_{n_i}(t)|^2$ constant, $H_{\rm int}$ is the interaction Hamiltonian and can increase or decrease one c^2 at the cost of others.

All operators who can change occupation numbers can be expressed in the operators a and $a^\dagger$. a is the *annihilation operator* and $a^\dagger$ the *creation operator*, and:

$$\begin{array}{rcl} a(\vec{k}_i)|n_1 n_2 \cdots n_i \cdots\rangle & = & \sqrt{n_i}\ |n_1 n_2 \cdots n_i - 1 \cdots\rangle \\ a^\dagger(\vec{k}_i)|n_1 n_2 \cdots n_i \cdots\rangle & = & \sqrt{n_i + 1}\ |n_1 n_2 \cdots n_i + 1 \cdots\rangle \end{array}$$

Because the states are normalized holds $a|0\rangle = 0$ and $a(\vec{k}_i)a^\dagger(\vec{k}_i)|n_i\rangle = n_i|n_i\rangle$. So $aa^\dagger$ is an occupation number operator. The following commutation rules can be derived:

$$[a(\vec{k}_i), a(\vec{k}_j)] = 0 \quad , \quad [a^\dagger(\vec{k}_i), a^\dagger(\vec{k}_j)] = 0 \quad , \quad [a(\vec{k}_i), a^\dagger(\vec{k}_j)] = \delta_{ij}$$

So for free spin-0 particles holds: $H_0 = \sum\limits_i a^\dagger(\vec{k}_i)a(\vec{k}_i)\hbar\omega_{k_i}$

15.2 Classical and quantum fields

Starting with a real field $\Phi^\alpha(x)$ (complex fields can be split in a real and an imaginary part), the *Lagrange density* $\mathcal{L}$ is a function of the position $x = (\vec{x}, ict)$ via the fields: $\mathcal{L} = \mathcal{L}(\Phi^\alpha(x), \partial_\nu\Phi^\alpha(x))$. The Lagrangian is given by $L = \int \mathcal{L}(x)d^3x$. Using the variational principle $\delta I(\Omega) = 0$ and with the action-integral $I(\Omega) = \int \mathcal{L}(\Phi^\alpha, \partial_\nu\Phi^\alpha)d^4x$ the field equation can be derived:

$$\frac{\partial\mathcal{L}}{\partial\Phi^\alpha} - \frac{\partial}{\partial x_\nu}\frac{\partial\mathcal{L}}{\partial(\partial_\nu\Phi^\alpha)} = 0$$

The *conjugated field* is, analogous with momentum in classical mechanics, defined as:

$$\Pi^\alpha(x)=\frac{\partial\mathcal{L}}{\partial\dot{\Phi}^\alpha}$$

With this, the Hamilton density becomes $\mathcal{H}(x)=\Pi^\alpha\dot{\Phi}^\alpha-\mathcal{L}(x)$.

Quantization of a classical field is analogous to quantization in point mass mechanics: the field functions are considered as operators obeying certain commutation rules:

$$[\Phi^\alpha(\vec{x}),\Phi^\beta(\vec{x}\,')]=0\quad,\quad[\Pi^\alpha(\vec{x}),\Pi^\beta(\vec{x}\,')]=0\quad,\quad[\Phi^\alpha(\vec{x}),\Pi^\beta(\vec{x}\,')]=i\delta_{\alpha\beta}(\vec{x}-\vec{x}\,')$$

15.3 The interaction picture

Some equivalent formulations of quantum mechanics are possible:

1. Schrödinger picture: time-dependent states, time-independent operators.
2. Heisenberg picture: time-independent states, time-dependent operators.
3. Interaction picture: time-dependent states, time-dependent operators.

The interaction picture can be obtained from the Schrödinger picture via an unitary transformation:

$$|\Phi(t)\rangle=\mathrm{e}^{iH_0^{\mathrm{S}}}|\Phi^{\mathrm{S}}(t)\rangle\ \text{ and }\ O(t)=\mathrm{e}^{iH_0^{\mathrm{S}}}O^{\mathrm{S}}\mathrm{e}^{-iH_0^{\mathrm{S}}}$$

The index $^{\mathrm{S}}$ denotes the Schrödinger picture. From this follows:

$$i\frac{d}{dt}|\Phi(t)\rangle=H_{\mathrm{int}}(t)|\Phi(t)\rangle\ \text{ and }\ i\frac{d}{dt}O(t)=[O(t),H_0]$$

15.4 Real scalar field in the interaction picture

It is easy to find that, with $M:=m_0^2c^2/\hbar^2$, holds:

$$\frac{\partial}{\partial t}\Phi(x)=\Pi(x)\ \text{ and }\ \frac{\partial}{\partial t}\Pi(x)=(\nabla^2-M^2)\Phi(x)$$

From this follows that Φ obeys the Klein-Gordon equation $(\Box-M^2)\Phi=0$. With the definition $k_0^2=\vec{k}^2+M^2:=\omega_k^2$ and the notation $\vec{k}\cdot\vec{x}-ik_0t:=kx$ the general solution of this equation is given by:

$$\Phi(x)=\frac{1}{\sqrt{V}}\sum_{\vec{k}}\frac{1}{\sqrt{2\omega_k}}\left(a(\vec{k})\mathrm{e}^{ikx}+a^\dagger(\vec{k})\mathrm{e}^{-ikx}\right)\quad;\quad\Pi(x)=\frac{i}{\sqrt{V}}\sum_{\vec{k}}\sqrt{\tfrac{1}{2}\omega_k}\left(-a(\vec{k})\mathrm{e}^{ikx}+a^\dagger(\vec{k})\mathrm{e}^{-ikx}\right)$$

The field operators contain a volume V, which is used as normalizing factor. Usually one can take the limit $V\to\infty$.

In general holds that the term with e^{-ikx}, the positive frequency part, is the creation part, and the negative frequency part is the annihilation part.

Because Φ is hermitian the coefficients have to be each others hermitian conjugate. Because Φ has only one component this can be interpreted as a field describing a particle with zero spin. From this follows that the commutation rules obey $[\Phi(x),\Phi(x')]=i\Delta(x-x')$ with

$$\Delta(y)=\frac{1}{(2\pi)^3}\int\frac{\sin(ky)}{\omega_k}d^3k$$

$\Delta(y)$ is a odd function which is invariant for proper Lorentz transformations (no mirroring). This is consistent with the previously found result $[\Phi(\vec{x},t,\Phi(\vec{x}\,',t)]=0$. In general holds that $\Delta(y)=0$ outside the light cone. So the equations obey the locality postulate.

The Lagrange density is given by: $\mathcal{L}(\Phi,\partial_\nu\Phi)=-\frac{1}{2}(\partial_\nu\Phi\partial_\nu\Phi+m^2\Phi^2)$. The energy operator is given by:

$$H=\int\mathcal{H}(x)d^3x=\sum_{\vec{k}}\hbar\omega_k a^\dagger(\vec{k})a(\vec{k})$$

15.5 Charged spin-0 particles, conservation of charge

The Lagrange density of charged spin-0 particles is given by: $\mathcal{L}=-(\partial_\nu\Phi\partial_\nu\Phi^*+M^2\Phi\Phi^*)$.

Noether's theorem connects a continuous symmetry of $\mathcal{L}$ and an additive conservation law. Suppose that $\mathcal{L}\left((\Phi^\alpha)',\partial_\nu(\Phi^\alpha)'\right)=\mathcal{L}\left(\Phi^\alpha,\partial_\nu\Phi^\alpha\right)$ and there exists a continuous transformation between Φ^α and $\Phi^{\alpha\prime}$ like $\Phi^{\alpha\prime}=\Phi^\alpha+\epsilon f^\alpha(\Phi)$. Then holds

$$\frac{\partial}{\partial x_\nu}\left(\frac{\partial\mathcal{L}}{\partial(\partial_\nu\Phi^\alpha)}f^\alpha\right)=0$$

This is a continuity equation ⇒ conservation law. Which quantity is conserved depends on the symmetry. The above Lagrange density is invariant for a change in phase $\Phi\rightarrow\Phi\mathrm{e}^{i\theta}$: a global gauge transformation. The conserved quantity is the current density $J_\mu(x)=-ie(\Phi\partial_\mu\Phi^*-\Phi^*\partial_\mu\Phi)$. Because this quantity is 0 for real fields a complex field is needed to describe charged particles. When this field is quantized the field operators are given by

$$\Phi(x)=\frac{1}{\sqrt{V}}\sum_{\vec{k}}\frac{1}{\sqrt{2\omega_k}}\left(a(\vec{k})\mathrm{e}^{ikx}+b^\dagger(\vec{k})\mathrm{e}^{-ikx}\right)\quad\text{and}\quad\Phi^\dagger(x)=\frac{1}{\sqrt{V}}\sum_{\vec{k}}\frac{1}{\sqrt{2\omega_k}}\left(a^\dagger(\vec{k})\mathrm{e}^{ikx}+b(\vec{k})\mathrm{e}^{-ikx}\right)$$

The energy operator is given by:

$$H=\sum_{\vec{k}}\hbar\omega_k\left(a^\dagger(\vec{k})a(\vec{k})+b^\dagger(\vec{k})b(\vec{k})\right)$$

and the charge operator follows from:

$$Q(t)=-i\int J_4(x)d^3x\Rightarrow Q=\sum_{\vec{k}}e\left(a^\dagger(\vec{k})a(\vec{k})-b^\dagger(\vec{k})b(\vec{k})\right)$$

From this follows that $a^\dagger a:=N_+(\vec{k})$ is an occupation number operator for particles with a positive charge and $b^\dagger b:=N_-(\vec{k})$ is an occupation number operator for particles with a negative charge.

15.6 Field functions for spin-$\frac{1}{2}$ particles

Spin is defined by the behaviour of the solutions ψ of the Dirac equation. A *scalar* field Φ has the property that if it obeys the Klein-Gordon equation also the rotated field $\tilde{\Phi}(x):=\Phi(\Lambda^{-1}x)$ obeys it. Λ denotes 4-dimensional rotations: the proper Lorentz transformations. These can be written as:

$$\tilde{\Phi}(x)=\Phi(x)\mathrm{e}^{-i\vec{n}\cdot\vec{L}}\quad\text{with}\quad L_{\mu\nu}=-i\hbar\left(x_\mu\frac{\partial}{\partial x_\nu}-x_\nu\frac{\partial}{\partial x_\mu}\right)$$

For $\mu\leq3,\nu\leq3$ this are rotations, for $\nu=4,\mu\neq4$ this are Lorentz transformations.

A rotated field $\tilde{\psi}$ obeys the Dirac equation if the following holds: $\tilde{\psi}(x)=D(\Lambda)\psi(\Lambda^{-1}x)$. This results in the condition $D^{-1}\gamma_\lambda D=\Lambda_{\lambda\mu}\gamma_\mu$. One finds: $D=\mathrm{e}^{i\vec{n}\cdot\vec{S}}$ with $S_{\mu\nu}=-i\frac{1}{2}\hbar\gamma_\mu\gamma_\nu$. So:

$$\tilde{\psi}(x)=\mathrm{e}^{-i(S+L)}\psi(x)=\mathrm{e}^{-iJ}\psi(x)$$

The solutions of the Dirac equation are then given by:

$$\psi(x)=u^r_\pm(\vec{p}\,)\mathrm{e}^{-i(\vec{p}\cdot\vec{x}\pm Et)}$$

Here, r is an indication for the direction of the spin, and ± is the sign of the energy. With the notation $v^r(\vec{p}\,) = u^r_-(-\vec{p}\,)$ and $u^r(\vec{p}\,) = u^r_+(\vec{p}\,)$ one can write for the dot products of these spinors:

$$u^r_+(\vec{p}\,)u^{r'}_+(\vec{p}\,) = \frac{E}{M}\delta_{rr'} \ \ , \ \ u^r_-(\vec{p}\,)u^{r'}_-(\vec{p}\,) = \frac{E}{M}\delta_{rr'} \ \ , \ \ u^r_+(\vec{p}\,)u^{r'}_-(\vec{p}\,) = 0$$

Because of the factor E/M this is not relativistic invariant. A Lorentz-invariant dot product is defined by $\overline{a}b := a^\dagger\gamma_4 b$, where $\overline{a} := a^\dagger\gamma_4$ is a row spinor. From this follows:

$$\overline{u^r(\vec{p}\,)}u^{r'}(\vec{p}\,) = \delta_{rr'} \ \ , \ \ \overline{v^r(\vec{p}\,)}v^{r'}(\vec{p}\,) = -\delta_{rr'} \ \ , \ \ \overline{u^r(\vec{p}\,)}v^{r'}(\vec{p}\,) = 0$$

Combinations of the type $a\overline{a}$ give a 4×4 matrix:

$$\sum_{r=1}^{2} u^r(\vec{p}\,)\overline{u^r(\vec{p}\,)} = \frac{-i\gamma_\lambda p_\lambda + M}{2M} \ \ , \ \ \sum_{r=1}^{2} v^r(\vec{p}\,)\overline{v^r(\vec{p}\,)} = \frac{-i\gamma_\lambda p_\lambda - M}{2M}$$

The Lagrange density resulting in the Dirac equation and has the correct energy normalization is:

$$\mathcal{L}(x) = -\overline{\psi(x)}\left(\gamma_\mu\frac{\partial}{\partial x_\mu} + M\right)\psi(x)$$

and the current density is $J_\mu(x) = -ie\overline{\psi}\gamma_\mu\psi$.

15.7 Quantization of spin-$\frac{1}{2}$ fields

The general solution for the fieldoperators is in this case:

$$\psi(x) = \sqrt{\frac{M}{V}}\sum_{\vec{p}}\frac{1}{\sqrt{E}}\sum_r\left(c_r(\vec{p}\,)u^r(\vec{p}\,)\mathrm{e}^{ipx} + d^\dagger_r(\vec{p}\,)v^r(\vec{p}\,)\mathrm{e}^{-ipx}\right)$$

and

$$\overline{\psi(x)} = \sqrt{\frac{M}{V}}\sum_{\vec{p}}\frac{1}{\sqrt{E}}\sum_r\left(c^\dagger_r(\vec{p}\,)\overline{u^r}(\vec{p}\,)\mathrm{e}^{-ipx} + d_r(\vec{p}\,)\overline{v^r}(\vec{p}\,)\mathrm{e}^{ipx}\right)$$

Here, $c^\dagger$ and c are the creation e.g. annihilation operators for an electron and $d^\dagger$ and d the creation e.g. annihilation operators for a positron. The energy operator is given by

$$H = \sum_{\vec{p}} E_{\vec{p}}\sum_{r=1}^{2}\left(c^\dagger_r(\vec{p}\,)c_r(\vec{p}\,) - d_r(\vec{p}\,)d^\dagger_r(\vec{p}\,)\right)$$

To prevent that the energy of positrons is negative the operators must obey anti commutation rules in stead of commutation rules:

$$[c_r(\vec{p}\,), c^\dagger_{r'}(\vec{p}\,)]_+ = [d_r(\vec{p}\,), d^\dagger_{r'}(\vec{p}\,)]_+ = \delta_{rr'}\delta_{pp'} \ \ , \ \ \text{all other anti commutators are 0.}$$

The field operators obey

$$[\psi_\alpha(x), \psi_\beta(x')] = 0 \ \ , \ \ [\overline{\psi_\alpha(x)}, \overline{\psi_\beta(x')}] = 0 \ \ , \ \ [\psi_\alpha(x), \overline{\psi_\beta(x')}]_+ = -iS_{\alpha\beta}(x - x')$$

$$\text{with} \quad S(x) = \left(\gamma_\lambda\frac{\partial}{\partial x_\lambda} - M\right)\Delta(x)$$

The anti commutation rules give except the positive-definite energy also the Pauli exclusion principle and the Fermi-Dirac statistics: because $c^\dagger_r(\vec{p}\,)c^\dagger_r(\vec{p}\,) = -c^\dagger_r(\vec{p}\,)c^\dagger_r(\vec{p}\,)$ holds: $\{c^\dagger_r(p)\}^2 = 0$. It appears to be not possible to create two electrons with the same momentum and spin. This is the exclusion principle. An other method to see this is the fact that $\{N^+_r(\vec{p}\,)\}^2 = N^+_r(\vec{p}\,)$: the occupation operators have only eigenvalues 0 and 1.

To avoid infinite vacuum contributions to the energy and charge the *normal product* is introduced. The expression for the current density now becomes $J_\mu = -ieN(\overline{\psi}\gamma_\mu\psi)$. This product is obtained by:

- Expand all fields to creation and annihilation operators,
- Keep all terms who have no annihilation operators, or in which they are at the right of the creation operators,
- In all other terms interchange the factors so that the annihilation operators go to the right. By an interchange of two fermion operators add a $-$ sign, by interchange of two boson operators not. Assume hereby that all commutators are 0.

15.8 Quantization of the electromagnetic field

Starting with the Lagrange density $\mathcal{L} = -\frac{1}{2}\frac{\partial A_\nu}{\partial x_\mu}\frac{\partial A_\nu}{\partial x_\mu}$

follows for the field operators $A(x)$:

$$A(x) = \frac{1}{\sqrt{V}}\sum_{\vec{k}}\frac{1}{\sqrt{2\omega_k}}\sum_{m=1}^{4}\left(a_m(\vec{k})\epsilon^m(\vec{k})\mathrm{e}^{ikx} + a^\dagger(\vec{k})\epsilon^m(\vec{k})^*\mathrm{e}^{-ikx}\right)$$

The operators obey $[a_m(\vec{k}), a^\dagger_{m'}(\vec{k})] = \delta_{mm'}\delta_{kk'}$. All other commutators are 0. m gives the polarization direction of the photon: $m = 1, 2$ gives transversal polarized, $m = 3$ longitudinal polarized and $m = 4$ timelike polarized photons. Further holds:

$$[A_\mu(x), A_\nu(x')] = i\delta_{\mu\nu}D(x - x') \quad \text{with} \quad D(y) = \Delta(y)|_{m=0}$$

In spite of the fact that $A_4 = iV$ is imaginary in the classical case, A_4 is still defined to be hermitian because otherwise the sign of the energy becomes incorrect. By changing the definition of the inner product in configuration space the expectation values for $A_{1,2,3}(x) \in I\!R$ and for $A_4(x)$ imaginary.

If the potentials satisfy the Lorentz gauge condition $\partial_\mu A_\mu = 0$ the E and B operators derived from these potentials will satisfy the Maxwell equations. However, this gives problems with the commutation rules. There is now demanded that only those states are permitted for which holds

$$\frac{\partial A^+_\mu}{\partial x_\mu}|\Phi\rangle = 0$$

This results in: $$\left\langle\frac{\partial A_\mu}{\partial x_\mu}\right\rangle = 0.$$

From this follows that $(a_3(\vec{k}) - a_4(\vec{k}))|\Phi\rangle = 0$. With a local gauge transformation one obtains $N_3(\vec{k}) = 0$ and $N_4(\vec{k}) = 0$. However, this only applies for free EM-fields: in intermediary states in interactions there can exist longitudinal and timelike photons. These photons are also responsible for the stationary Coulomb potential.

15.9 Interacting fields and the S-matrix

The S(scattering)-matrix gives a relation between the initial and final states for an interaction: $|\Phi(\infty)\rangle = S|\Phi(-\infty)\rangle$. If the Schrödinger equation is integrated:

$$|\Phi(t)\rangle = |\Phi(-\infty)\rangle - i\int\limits_{-\infty}^{t} H_{\text{int}}(t_1)|\Phi(t_1)\rangle dt_1$$

and perturbation theory is applied one finds that:

$$S = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int\cdots\int T\left\{\mathcal{H}_{\text{int}}(x_1)\cdots\mathcal{H}_{\text{int}}(x_n)\right\}d^4x_1\cdots d^4x_n \equiv \sum_{n=0}^{\infty}S^{(n)}$$

Here, the T-operator means a *time-ordened product*: the terms in such a product must be oredned in increasing time order from the right to the left so that the earliest terms work first. The S-matrix is then given by: $S_{ij} = \langle\Phi_i|S|\Phi_j\rangle = \langle\Phi_i|\Phi(\infty)\rangle$.

The interaction Hamilton density for the interaction between the electromagnetic and the electron-positron field is: $\mathcal{H}_{\rm int}(x) = -J_\mu(x)A_\mu(x) = ieN(\overline{\psi}\gamma_\mu\psi A_\mu)$

When this is expanded as: $\mathcal{H}_{\rm int} = ieN\left((\overline{\psi^+} + \overline{\psi^-})\gamma_\mu(\psi^+ + \psi^-)(A_\mu^+ + A_\mu^-)\right)$

eight terms appear. Each term corresponds with a possible process. The term $ie\overline{\psi^+}\gamma_\mu\psi^+A_\mu^-$ working on $|\Phi\rangle$ gives transitions where A_μ^- creates a photon, ψ^+ annihilates an electron and $\overline{\psi^+}$ annihilates a positron. Only terms with the correct number of particles in the initial and final state contribute to a matrixelement $\langle\Phi_i|S|\Phi_j\rangle$. Further the factors in $\mathcal{H}_{\rm int}$ can create and thereafter annihilate particles: the *virtual particles*.

The expressions for $S^{(n)}$ contain time-ordened products of normal products. This can be written as a sum of normal products. The appearing operators describe the minimal changes necessary to change the initial state in the final state. The effects of the virtual particles are described by the (anti)commutator functions. Some time-ordened products are:

$$\begin{array}{rcl}
T\left\{\Phi(x)\Phi(y)\right\} &=& N\left\{\Phi(x)\Phi(y)\right\} + \frac{1}{2}\Delta^{\rm F}(x-y)\\
T\left\{\psi_\alpha(x)\overline{\psi_\beta(y)}\right\} &=& N\left\{\psi_\alpha(x)\overline{\psi_\beta(y)}\right\} - \frac{1}{2}S^{\rm F}_{\alpha\beta}(x-y)\\
T\left\{A_\mu(x)A_\nu(y)\right\} &=& N\left\{A_\mu(x)A_\nu(y)\right\} + \frac{1}{2}\delta_{\mu\nu}D^{\rm F}_{\mu\nu}(x-y)
\end{array}$$

Here, $S^{\rm F}(x) = (\gamma_\mu\partial_\mu - M)\Delta^{\rm F}(x)$, $D^{\rm F}(x) = \Delta^{\rm F}(x)|_{m=0}$ and

$$\Delta^{\rm F}(x) = \left\{\begin{array}{ll}
\displaystyle\frac{1}{(2\pi)^3}\int\frac{{\rm e}^{ikx}}{\omega_{\vec{k}}}d^3k & \text{if } x_0 > 0\\[2ex]
\displaystyle\frac{1}{(2\pi)^3}\int\frac{{\rm e}^{-ikx}}{\omega_{\vec{k}}}d^3k & \text{if } x_0 < 0
\end{array}\right.$$

The term $\frac{1}{2}\Delta^{\rm F}(x-y)$ is called the contraction of $\Phi(x)$ and $\Phi(y)$, and is the expectation value of the time-ordened product in the vacuum state. Wick's theorem gives an expression for the time-ordened product of an arbitrary number of field operators. The graphical representation of these processes are called *Feynman diagrams*. In the x-representation each diagram describes a number of processes. The contraction functions can also be written as:

$$\Delta^{\rm F}(x) = \lim_{\epsilon\to0}\frac{-2i}{(2\pi)^4}\int\frac{{\rm e}^{ikx}}{k^2+m^2-i\epsilon}d^4k \quad\text{and}\quad S^{\rm F}(x) = \lim_{\epsilon\to0}\frac{-2i}{(2\pi)^4}\int{\rm e}^{ipx}\frac{i\gamma_\mu p_\mu - M}{p^2+M^2-i\epsilon}d^4p$$

In the expressions for $S^{(2)}$ this gives rise to terms $\delta(p+k-p'-k')$. This means that energy and momentum is conserved. However, virtual particles do not obey the relation between energy and momentum.

15.10 Divergences and renormalization

It turns out that higher order contribute infinitely much because only the sum $p+k$ of the four-momentum of the virtual particles is fixed. An integration over one of both becomes ∞. In the x-representation this can be understood because the product of two functions containing δ-like singularities is not well defined. This is solved by discounting all divergent diagrams in a renormalization of e and M. It is assumed that an electron, if there would not be an electromagnetical field, would have a mass M_0 and a charge e_0 unequal to the observed mass M and charge e. In the Hamilton and Lagrange density of the free electron-positron field appears M_0. So this gives, with $M = M_0 + \Delta M$:

$$\mathcal{L}_{\rm e-p}(x) = -\overline{\psi(x)}(\gamma_\mu\partial_\mu + M_0)\psi(x) = -\overline{\psi(x)}(\gamma_\mu\partial_\mu + M)\psi(x) + \Delta M\overline{\psi(x)}\psi(x)$$

and $\mathcal{H}_{\rm int} = ieN(\overline{\psi}\gamma_\mu\psi A_\mu) - i\Delta eN(\overline{\psi}\gamma_\mu\psi A_\mu)$.

15.11 Classification of elementary particles

Elementary particles can be categorized as follows:

1. **Hadrons:** these exists of quarks, and can be categorized in:
    - I. **Baryons:** these exists of 3 quarks or 3 antiquarks.
    - II. **Mesons:** these exists of one quark and one antiquark.
2. **Leptons:** $\mathrm{e}^\pm$, $\mu^\pm$, $\tau^\pm$, ν_e, ν_μ, ν_τ, $\overline{\nu}_\mathrm{e}$, $\overline{\nu}_\mu$, $\overline{\nu}_\tau$.
3. **Field quanta:** γ, $\mathrm{W}^\pm$, Z^0, gluons, gravitons (?).

An overview is given in the following table:

Particle	spin ($\hbar$)	B	L	T	T_3	S	C	B*	charge (e)	m_0 (MeV)	antipart.
u	$\pm1/2$	1/3	0	1/2	1/2	0	0	0	2/3	5	$\overline{\mathrm{u}}$
d	$\pm1/2$	1/3	0	1/2	$-1/2$	0	0	0	$-1/3$	8	$\overline{\mathrm{d}}$
s	$\pm1/2$	1/3	0	0	0	-1	0	0	$-1/3$	175	$\overline{\mathrm{s}}$
c	$\pm1/2$	1/3	0	0	0	0	1	0	2/3	1270	$\overline{\mathrm{c}}$
b	$\pm1/2$	1/3	0	0	0	0	0	-1	$-1/3$	4200	$\overline{\mathrm{b}}$
t	$\pm1/2$	1/3	0	0	0	0	0	0	2/3	170000	$\overline{\mathrm{t}}$
e^-	$\pm1/2$	0	1	0	0	0	0	0	-1	0,511	e^+
μ^-	$\pm1/2$	0	1	0	0	0	0	0	-1	105,7	μ^+
τ^-	$-1/2$	0	1	0	0	0	0	0	-1	1784	τ^+
ν_e	$-1/2$	0	1	0	0	0	0	0	0	0(?)	$\overline{\nu}_\mathrm{e}$
ν_μ	$-1/2$	0	1	0	0	0	0	0	0	0(?)	$\overline{\nu}_\mu$
ν_τ	$-1/2$	0	1	0	0	0	0	0	0	0(?)	$\overline{\nu}_\tau$

Where B is the baryon number and L the lepton number. It is found that there are three different lepton numbers, one for e, μ and τ. T is the isospin, with T_3 the projection of the isospin on the third axis, C the charmness, S the strangeness and B* the bottomness. The anti particles have quantum numbers with the opposite sign except for the total isospin T. The hadrons are as follows composed from (anti)quarks:

π^0	$\frac{1}{2}\sqrt{2}(\mathrm{u}\overline{\mathrm{u}}+\mathrm{d}\overline{\mathrm{d}})$	J/Ψ	$\mathrm{c}\overline{\mathrm{c}}$	$\overline{\Sigma^+}$	$\overline{\mathrm{d}}\ \overline{\mathrm{d}}\ \overline{\mathrm{s}}$
π^+	$\mathrm{u}\overline{\mathrm{d}}$	T	$\mathrm{b}\overline{\mathrm{b}}$	Ξ^0	u s s
π^-	$\mathrm{d}\overline{\mathrm{u}}$	p^+	u u d	$\overline{\Xi}^0$	$\overline{\mathrm{u}}\ \overline{\mathrm{s}}\ \overline{\mathrm{s}}$
K^0	$\mathrm{s}\overline{\mathrm{d}}$	p^-	$\overline{\mathrm{u}}\ \overline{\mathrm{u}}\ \overline{\mathrm{d}}$	Ξ^-	d s s
K^0	$\mathrm{d}\overline{\mathrm{s}}$	n^0	u d d	Ξ^+	$\overline{\mathrm{d}}\ \overline{\mathrm{s}}\ \overline{\mathrm{s}}$
K^+	$\mathrm{u}\overline{\mathrm{s}}$	$\overline{\mathrm{n}}^0$	$\overline{\mathrm{u}}\ \overline{\mathrm{d}}\ \overline{\mathrm{d}}$	Ω^-	s s s
K^-	$\mathrm{s}\overline{\mathrm{u}}$	Λ	u d s	Ω^+	$\overline{\mathrm{s}}\ \overline{\mathrm{s}}\ \overline{\mathrm{s}}$
D^+	$\mathrm{c}\overline{\mathrm{d}}$	$\overline{\Lambda}$	$\overline{\mathrm{u}}\ \overline{\mathrm{d}}\ \overline{\mathrm{s}}$	Λ_c^+	u d c
D^-	$\mathrm{d}\overline{\mathrm{c}}$	Σ^+	u u s	Δ^{2-}	$\overline{\mathrm{u}}\ \overline{\mathrm{u}}\ \overline{\mathrm{u}}$
D^0	$\mathrm{c}\overline{\mathrm{u}}$	$\overline{\Sigma^-}$	$\overline{\mathrm{u}}\ \overline{\mathrm{u}}\ \overline{\mathrm{s}}$	Δ^{2+}	u u u
D^0	$\mathrm{u}\overline{\mathrm{c}}$	Σ^0	u d s	Δ^+	u u d
F^+	$\mathrm{c}\overline{\mathrm{s}}$	Σ^0	$\overline{\mathrm{u}}\ \overline{\mathrm{d}}\ \overline{\mathrm{s}}$	Δ^0	u d d
F^-	$\mathrm{s}\overline{\mathrm{c}}$	Σ^-	d d s	Δ^-	d d d

Each quark can exist is two spin states. So mesons are bosons with spin 0 or ±1 while baryons are fermions with spin $\pm\frac{1}{2}$ or $\pm\frac{3}{2}$.

The quantum numbers are subject to conservation laws. These can be derived from symmetries in the Lagrange density: continuous symmetries give rise to additive conservation laws, discrete symmetries result in multiplicative conservation laws.

Geometrical conservation laws are invariant under Lorentz transformations and the CPT-operation. These are:

1. Mass/energy because the laws of nature are invariant for translations in time.
2. Momentum because the laws of nature are invariant for translations in space.
3. Angular momentum because the laws of nature are invariant for rotations.

Dynamical conservation laws are invariant under the CPT-operation. These are:

1. Electrical charge because the Maxwell equations are invariant under gauge transformations.
2. Color charge is conserved.
3. Isospin because QCD is invariant for rotations in T-space.
4. Baryon number and lepton number are conserved but not under a possible SU(5) symmetry of the laws of nature.
5. Quarks type is only conserved under the color interaction.
6. Parity is conserved except for weak interactions.

The elementary particles can be classified into three families:

	leptons	quarks	antileptons	antiquarks
1st generation	e^- ν_e	d u	e^+ $\overline{\nu}_\mathrm{e}$	$\overline{\mathrm{d}}$ $\overline{\mathrm{u}}$
2nd generation	μ^- ν_μ	s c	μ^+ $\overline{\nu}_\mu$	$\overline{\mathrm{s}}$ $\overline{\mathrm{c}}$
3rd generation	τ^- ν_τ	b t	τ^+ $\overline{\nu}_\tau$	$\overline{\mathrm{b}}$ $\overline{\mathrm{t}}$

Quarks exist in three colors but because they are *confined* these colors can not be seen directly. The color force does *not* decrease with distance. The potential energy shall be high enough to create a quark-antiquark pair when it is tried to free an (anti)quark from a hadron. This will result in two hadrons and not in free quarks.

15.12 P and CP-violation

It is found that the weak interaction violates P-symmetry, and even CP-symmetry is not conserved. Some processes which violate P symmetry but conserve the combination CP are:

1. μ-decay: $\mu^- \rightarrow \mathrm{e}^- + \nu_\mu + \overline{\nu}_\mathrm{e}$. Left-handed electrons appear more than 1000× as much as right-handed ones.
2. β-decay of spin-polarized ^{60}Co: $^{60}\mathrm{Co} \rightarrow ^{60}\mathrm{Ni} + \mathrm{e}^- + \overline{\nu}_\mathrm{e}$. More electrons with a spin parallel to the Co than with a spin antiparallel are created: (parallel−antiparallel)/(total)=20%.
3. There is no connection with the neutrino: the decay of the Λ particle via: $\Lambda \rightarrow \mathrm{p}^+ + \pi^-$ and $\Lambda \rightarrow \mathrm{n}^0 + \pi^0$ has also these properties.

The CP-symmetry was found to be violated at the decay of neutral Kaons. This are the lowest possible states with a s-quark so they can decay only weak. The following holds: $\mathrm{C}|\mathrm{K}^0\rangle = \eta|\overline{\mathrm{K}^0}\rangle$ where η is a phase factor. Further holds $\mathrm{P}|\mathrm{K}^0\rangle = -|\mathrm{K}^0\rangle$ because K^0 and $\overline{\mathrm{K}^0}$ have an intrinsic parity of -1. From this follows that K^0 and $\overline{\mathrm{K}^0}$ are not eigenvalues of CP: $\mathrm{CP}|\mathrm{K}^0\rangle = |\overline{\mathrm{K}^0}\rangle$. The linear combinations

$$|\mathrm{K}^0_1\rangle := \tfrac{1}{2}\sqrt{2}(|\mathrm{K}^0\rangle + |\overline{\mathrm{K}^0}\rangle) \quad \text{and} \quad |\mathrm{K}^0_2\rangle := \tfrac{1}{2}\sqrt{2}(|\mathrm{K}^0\rangle - |\overline{\mathrm{K}^0}\rangle)$$

are eigenstates of CP: $\mathrm{CP}|\mathrm{K}^0_1\rangle = +|\mathrm{K}^0_1\rangle$ and $\mathrm{CP}|\mathrm{K}^0_2\rangle = -|\mathrm{K}^0_2\rangle$. A base of K^0_1 and K^0_2 is practical while describing weak interactions. For color interactions a base of K^0 and $\overline{\mathrm{K}^0}$ is practical because then the number u−number $\overline{\mathrm{u}}$ is constant. The expansion postulate must be used for weak decays:

$$|\mathrm{K}^0\rangle = \tfrac{1}{2}(\langle\mathrm{K}^0_1|\mathrm{K}^0\rangle + \langle\mathrm{K}^0_2|\mathrm{K}^0\rangle)$$

The probability to find a final state with CP$=-1$ is $\frac{1}{2}|\left\langle \mathrm{K}_2^0|\mathrm{K}^0\right\rangle|^2$, the probability on CP=+1 decay is $\frac{1}{2}|\left\langle \mathrm{K}_1^0|\mathrm{K}^0\right\rangle|^2$.

The relation between the mass eigenvalues of the quarks (unaccented) and the fields arising in the weak currents (accented) is $(u', c', t') = (u, c, t)$, and:

$$
\begin{aligned}
\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_2 & \sin\theta_2 \\ 0 & -\sin\theta_2 & \cos\theta_2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathrm{e}^{i\delta} \end{pmatrix} \begin{pmatrix} \cos\theta_1 & \sin\theta_1 & 0 \\ -\sin\theta_1 & \cos\theta_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
& \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_3 & \sin\theta_3 \\ 0 & -\sin\theta_3 & \cos\theta_3 \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}
\end{aligned}
$$

$\theta_1 \equiv \theta_\mathrm{C}$ is the *Cabibbo angle*: $\sin(\theta_\mathrm{C}) \approx 0,23 \pm 0,01$.

15.13 The standard model

When one wants to make the Lagrange density which describes a field invariant for local gauge transformations from a certain group one has to perform the transformation

$$\frac{\partial}{\partial x_\mu} \rightarrow \frac{D}{Dx_\mu} = \frac{\partial}{\partial x_\mu} - i\frac{g}{\hbar}L_k A_\mu^k$$

Here the L_k are the generators of the gauge group (the "charges") and the A_μ^k are the gauge fields. g is the applying coupling constant. The Lagrange density for a scalar field becomes:

$$\mathcal{L} = -\tfrac{1}{2}(D_\mu\Phi^* D^\mu\Phi + M^2\Phi^*\Phi) - \tfrac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu}$$

and the field tensors are given by: $F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + gc_{lm}^a A_\mu^l A_\nu^m$.

15.13.1 The electroweak theory

The electroweak interaction arises from the necessity to keep the Lagrange density invariant for local gauge transformations of the group SU(2)⊗U(1). Right and left-handed spin states are treated different because the weak interaction does not conserve parity. If a fifth Dirac matrix is defined by:

$$\gamma_5 := \gamma_1\gamma_2\gamma_3\gamma_4 = -\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

the left and right handed solutions of the Dirac equation for neutrino's are given by:

$$\psi_\mathrm{L} = \tfrac{1}{2}(1+\gamma_5)\psi \quad \text{and} \quad \psi_\mathrm{R} = \tfrac{1}{2}(1-\gamma_5)\psi$$

It appears that neutrino's are always left-handed while antineutrino's are always right-handed. The *hypercharge* Y, for quarks given by $Y = \mathrm{B}+\mathrm{S}+\mathrm{C}+\mathrm{B}^*+\mathrm{T}'$, is defined by:

$$Q = \tfrac{1}{2}Y + T_3$$

so $[Y, T_k] = 0$. The group $\mathrm{U}(1)_Y \otimes \mathrm{SU}(2)_T$ is taken as symmetry group for the electroweak interaction because the generators of this group commute. The multiplets are classified as follows:

	e_R^-	ν_{eL} e_L^-	u_L d'_L	u_R	d_R
T	0	$\frac{1}{2}$	$\frac{1}{2}$	0	0
T_3	0	$\frac{1}{2}$ $-\frac{1}{2}$	$\frac{1}{2}$ $-\frac{1}{2}$	0	0
Y	-2	-1	$\frac{1}{3}$	$\frac{4}{3}$	$-\frac{2}{3}$

Now, 1 field $B_\mu(x)$ is connected with gauge group U(1) and 3 gauge fields $\vec{A}_\mu(x)$ are connected with SU(2). The total Lagrange density (minus the fieldterms) for a scalar field now becomes:

$$\begin{array}{rcl}\mathcal{L}_{0,\rm EZ} & = & -(\overline{\psi_{\nu\rm e,L}},\overline{\psi_{\rm eL}})\gamma^\mu\left(\partial_\mu - i\frac{g}{\hbar}\vec{A}_\mu\cdot(\frac{1}{2}\vec{\sigma}) - \frac{1}{2}i\frac{g'}{\hbar}B_\mu\cdot(-1)\right)\left(\begin{array}{c}\psi_{\nu\rm e,L}\\ \psi_{\rm eL}\end{array}\right) - \\ & & \overline{\psi_{\rm eR}}\gamma^\mu\left(\partial_\mu - \frac{1}{2}i\frac{g'}{\hbar}(-2)B_\mu\right)\psi_{\rm eR}\end{array}$$

Here, $\frac{1}{2}\vec{\sigma}$ are the generators of T and -1 and -2 the generators of Y.

15.13.2 Spontaneous symmetry breaking

All leptons are massless in the equations above. Their mass is probably generated by *spontaneous symmetry breaking*. This means that the dynamic equations which describe the system have a symmetry which the ground state does not have. It is assumed that there exist an isospin-doublet of scalar fields Φ with electrical charges +1 and 0. (Their antiparticles have charges −1 and 0). The extra terms in $\mathcal{L}$ arising from these fields are globally U(1)⊗SU(2) symmetrical. Further it is assumed that the state with the lowest energy corresponds with the state $\Phi(x)$ =constant. The state on which the system fluctuates is chosen so that

$$\langle\Phi\rangle = \left(\begin{array}{c}\langle\Phi^+\rangle\\ \langle\Phi^0\rangle\end{array}\right) = \left(\begin{array}{c}0\\ \langle v\rangle\end{array}\right)$$

Because of this expectation value $\neq 0$ the SU(2) symmetry is broken but the U(1) symmetry is not. When the gaugefields in the resulting Lagrange density are separated one obtains:

$$\begin{array}{rcl}W_\mu^- & = & \frac{1}{2}\sqrt{2}(A_\mu^1 + iA_\mu^2)\ \ ,\ \ W_\mu^+ \ = \ \frac{1}{2}\sqrt{2}(A_\mu^1 - iA_\mu^2)\\ Z_\mu & = & \dfrac{gA_\mu^3 - g'B_\mu}{\sqrt{g^2+g'^2}} \equiv A_\mu^3\cos(\theta_{\rm W}) - B_\mu\sin(\theta_{\rm W})\\ A_\mu & = & \dfrac{g'A_\mu^3 + gB_\mu}{\sqrt{g^2+g'^2}} \equiv A_\mu^3\sin(\theta_{\rm W}) + B_\mu\cos(\theta_{\rm W})\end{array}$$

where $\theta_{\rm W}$ is called the *Weinberg angle*. For this angle holds: $\sin^2(\theta_{\rm W}) = 0,255 \pm 0,010$. From the remaining terms can relations for the masses of the field quanta be obtained: $M_W = \frac{1}{2}vg$ and $M_Z = \frac{1}{2}v\sqrt{g^2+g'^2}$, and for the elementary charge holds: $e = \dfrac{gg'}{\sqrt{g^2+g'^2}} = g'\cos(\theta_{\rm W}) = g\sin(\theta_{\rm W})$

Experimentally it is found that $M_W = 80,9 \pm 1,5$ GeV/c^2 and $M_Z = 95,6 \pm 1,4$ GeV/c^2. according to the weak theory this should be: $M_W = 83,0 \pm 0,24$ GeV/c^2 and $M_Z = 93,8 \pm 2,0$ GeV/c^2.

15.13.3 Quantumchromodynamics

Colored particles interact because the Lagrange density is invariant for the transformations of the group SU(3) of the color interaction. A distinction can be made between two kinds of particles:

1. "White" particles: they have no color charge, the generator $\vec{T} = 0$.
2. "Colored" particles: the generators $\vec{T}$ are 8 3×3 matrices. There exist three colors and three anticolors.

The Lagrange density for colored particles is given by

$$\mathcal{L}_{\rm QCD} = i\sum_k \overline{\Psi_k}\gamma^\mu D_\mu\Psi_k + \sum_{k,l}\overline{\Psi_k}M_{kl}\Psi_l - \frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu}$$

The gluons remain massless because this Lagrange density does not contain spinless particles. Because left- and right handed quarks now belong to the same multiplet a mass term can be introduced. This term can be brought in the form $M_{kl} = m_k\delta_{kl}$.

15.14 Pathintegrals

The development in time of a quantummechanical system can, except with Schrödingers equation, also be described with a *pathintegral* (Feynman):

$$\psi(x',t')=\int F(x',t',x,t)\psi(x,t)dx$$

in which $F(x',t',x,t)$ is the amplitude of probability to find a system on time t' in x' if it was in x on time t. Then,

$$F(x',t',x,t)=\int\exp\left(\frac{iS[x]}{\hbar}\right)d[x]$$

where $S[x]$ is an action-integral: $S[x]=\int L(x,\dot{x},t)dt$. The notation $d[x]$ means that the integral has to be taken over all possible paths $[x]$:

$$\int d[x]:=\lim_{n\to\infty}\frac{1}{N}\prod_n\left\{\int\limits_{-\infty}^{\infty}dx(t_n)\right\}$$

in which N a normalization constant is. To each path is assigned a probability amplitude $\exp(iS/\hbar)$. The classical limit can be found by taking $\delta S=0$: the average of the exponent vanishes, except where he is stationary. In quantumvfieldtheory, the probability of the transition of a fieldoperator $\Phi(\vec{x},-\infty)$ to $\Phi'(\vec{x},\infty)$ is given by

$$F(\Phi'(\vec{x},\infty),\Phi(\vec{x},-\infty))=\int\exp\left(\frac{iS[\Phi]}{\hbar}\right)d[\Phi]$$

with the action-integral

$$S[\Phi]=\int\limits_{\Omega}\mathcal{L}(\Phi,\partial_\nu\Phi)d^4x$$

Chapter 16

Astrophysics

16.1 Determination of distances

To determine distances in the near space, the *parallax* is mostly used. The parallax is the angular difference between two measurements of the position of the object from different views. If the annual parallax is given by p, the distance R of the object is given by $R = a/\sin(p)$, in which a is the radius of Earth's orbit. The *clusterparallax* is used to determine the distance of a group of stars by using their motion w.r.t a fixed background. The tangential velocity v_t and the radial velocity v_r of the stars along the sky are given by

$$v_\mathrm{r} = V\cos(\theta) \quad , \quad v_\mathrm{t} = V\sin(\theta) = \omega R$$

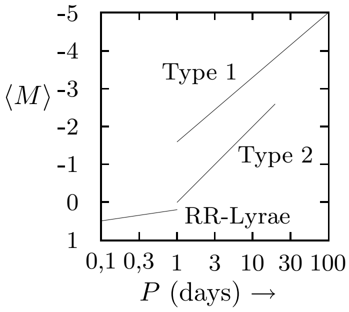
where θ is the angle between the star and the *point of convergence* and $\hat{R}$ the distance in pc. This results, with $v_\mathrm{t} = v_\mathrm{r}\tan(\theta)$, in:

$$R = \frac{v_\mathrm{r}\tan(\theta)}{\omega} \ \Rightarrow\ \hat{R} = \frac{1''}{p}$$

where p is the parallax in arch seconds. The parallax is then given by

$$p = \frac{4,74\mu}{v_\mathrm{r}\tan(\theta)}$$

with μ de self motion of the star in $''$/yr. A method to determine the distance of objects which are somewhat further away, like galaxies and star clusters, uses the period-Brightness relation between Cepheids. This relation is shown in the above figure for different types of stars.



16.2 Brightnes and magnitudes

The *brightness* is the total radiated energy per unit of time. Earth receives $s_0 = 1,374$ kW/m^2 from the Sun. So, the brightness of the Sun is given by $L_\odot = 4\pi r^2 s_0 = 3,82 \cdot 10^{26}$ W. It is also given by:

$$L_\odot = 4\pi R_\odot^2 \int\limits_0^\infty \pi F_\nu d\nu$$

where πF_ν is the monochromatic radiation flux. On the position of an observer this is πf_ν, with $f_\nu = (R/r)^2 F_\nu$ if absorption is ignored. If the fraction of the flux which reaches Earth's surface is called A_ν, the transmission factor is given by R_ν and the surface of the detector is given by πa^2, the apparent brightness b is given by:

$$b = \pi a^2 \int\limits_0^\infty f_\nu A_\nu R_\nu d\nu$$

The *magnitude* m is defined by:

$$\frac{b_1}{b_2} = (100)^{\frac{1}{5}(m_2 - m_1)} = (2,512)^{m_2 - m_1}$$

because the human eye perceives lightintensities logaritmical. From this follows that $m_2 - m_1 = 2,5 \cdot{}^{10}\log(b_1/b_2)$, or: $m = -2,5 \cdot{}^{10}\log(b) + C$. The apparent brightness of a star if this star would be at a distance of 10 pc is called the *absolute brightness* B: $B/b = (\hat{r}/10)^2$. The absolute magnitude is then given by $M = -2,5 \cdot{}^{10}\log(B) + C$, or: $M = 5 + m - 5 \cdot{}^{10}\log(\hat{r})$. When an interstellar absorption of 10^{-4}/pc is taken into account one finds:

$$M = (m - 4 \cdot 10^{-4}\hat{r}) + 5 - 5 \cdot{}^{10}\log(\hat{r})$$

If a detector detects all radiation emitted by a source one would measure the *absolute bolometric magnitude*. If the *bolometric correction BC* is given by

$$BC = 2,5 \cdot{}^{10}\log\left(\frac{\text{Energy flux received}}{\text{Energy flux registered}}\right) = 2,5 \cdot{}^{10}\log\left(\frac{\int f_\nu d\nu}{\int f_\nu A_\nu R_\nu d\nu}\right)$$

holds: $M_b = M_V - BC$ where M_V is the visual magnitude. Further holds

$$M_b = -2,5 \cdot{}^{10}\log\left(\frac{L}{L_\odot}\right) + 4,72$$

16.3 Radiation and stellar atmospheres

The radiation energy passing through a surface dA is $dE = I_\nu(\theta\varphi)\cos(\theta)d\nu d\Omega dAdt$, where I_μ is the *monochromatical intensity* $[\text{Wm}^{-2}\text{sr}^{-1}\text{Hz}^{-1}]$. When there is no absorption is the quantity I_ν independent of the distance to the source. Planck's law holds for a black body:

$$I_\nu(T) \equiv B_\nu(T) = \frac{c}{4\pi}w_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{\exp(h\nu/kT) - 1}$$

The radiation transport through a layer can than be written as:

$$\frac{dI_\nu}{ds} = -I_\nu\kappa_\nu + j_\nu$$

Here, j_ν is the *coefficient of emission* and κ_ν the *coefficient of absorption*. $\int ds$ is the thickness of the layer. The *optical thickness* τ_ν of the layer is given by $\tau_\nu = \int \kappa_\nu ds$. The layer is optically thin if $\tau_\nu \ll 1$, the layer is optically thick as $\tau_\nu \gg 1$. For a stellar atmosphere in LTE holds: $j_\nu = \kappa_\nu B_\nu(T)$. Then also holds:

$$I_\nu(s) = I_\nu(0)\mathrm{e}^{-\tau_\nu} + B_\nu(T)(1 - \mathrm{e}^{-\tau_\nu})$$

16.4 Composition and evolution of stars

The construction of a star is described by the following equations:

$$\begin{aligned}
\frac{dM(r)}{dr} &= 4\pi\varrho(r)r^2 \\
\frac{dp(r)}{dr} &= -\frac{GM(r)\varrho(r)}{r^2} \\
\frac{L(r)}{dr} &= 4\pi\varrho(r)\varepsilon(r)r^2 \\
\left(\frac{dT(r)}{dr}\right)_{\text{stral}} &= -\frac{3}{4}\frac{L(r)}{4\pi r^2}\frac{\kappa(r)}{4\sigma T^3(r)}\ , \quad \text{(Eddington), or} \\
\left(\frac{dT(r)}{dr}\right)_{\text{conv}} &= \frac{T(r)}{p(r)}\frac{\gamma - 1}{\gamma}\frac{dp(r)}{dr}\ , \quad \text{(convective energy transport)}
\end{aligned}$$

Further, for stars of the solar type, the composing plasma can be described as an ideal gas:

$$p(r) = \frac{\varrho(r)kT(r)}{\mu m_{\mathrm{H}}}$$

where μ is the average molecular mass, usually well approximated by:

$$\mu=\frac{\varrho}{nm_{\rm H}}=\frac{1}{2X+\frac{3}{4}Y+\frac{1}{2}Z}$$

where X is the mass fraction of H is, Y the mass fraction of He and Z the mass fraction of the other elements. Further holds:

$$\kappa(r)=f(\varrho(r),T(r),\mbox{composition})\ \ \mbox{and}\ \ \varepsilon(r)=g(\varrho(r),T(r),\mbox{composition})$$

Convection will occur when the star meets the Schwartzschild criterium:

$$\left(\frac{dT}{dr}\right)_{\rm conv}<\left(\frac{dT}{dr}\right)_{\rm stral}$$

Otherwise the energy transfer shall be by radiation. For stars in quasi-hydrostatic equilibrium hold the approximations $r=\frac{1}{2}R$, $M(r)=\frac{1}{2}M$, $dM/dr=M/R$, $\kappa\sim\varrho$ and $\varepsilon\sim\varrho T^\mu$ (this last assumption is only valid for stars on the main sequence). For pp-chains holds $\mu\approx5$ and for the CNO chaines holds $\mu=12$ tot 18. It can be derived that $L\sim M^3$: the *mass-brightness relation.* Further holds: $L\sim R^4\sim T_{\rm eff}^8$. This results in the equation of the main sequence in the Hertzsprung-Russel diagram:

$$^{10}\log(L)=8\cdot{}^{10}\log(T_{\rm eff})+\mbox{constant}$$

16.5 Energy production in stars

The net reaction from which most stars gain their energy is: $4{}^1{\rm H}\to{}^4\,{\rm He}+2{\rm e}^++2\nu_{\rm e}+\gamma$.
This reaction produces 26,72 MeV. Two reaction chains are responsible for this reaction. The slowest, speed-limiting reaction is shown in boldface. The energy between brackets is the energy cried away by the neutrino.

1. The proton-proton chain can be divided in two subchains:
   $\mathbf{{}^1H+p^+\to{}^2\,D+e^++\boldsymbol{\nu}_e}$, and then ${}^2{\rm D}+{\rm p}\to{}^3\,{\rm He}+\gamma$.

   I. pp1: ${}^3{\rm He}+{}^3\,{\rm He}\to2{\rm p}^++{}^4\,{\rm He}$. There is 26,21 + (0,51) MeV released.

   II. pp2: ${}^3{\rm He}+\alpha\to{}^7\,{\rm Be}+\gamma$

      i. ${}^7{\rm Be}+{\rm e}^-\to{}^7{\rm Li}+\nu$, dan ${}^7{\rm Li}+{\rm p}^+\to2{}^4{\rm He}+\gamma$. 25,92 + (0,80) MeV.

      ii. ${}^7{\rm Be}+{\rm p}^+\to{}^8{\rm B}+\gamma$, dan ${}^8{\rm B}+{\rm e}^+\to2{}^4{\rm He}+\overline{\nu}$. 19,5 + (7,2) MeV.

      Both ^{7}Be chains become more important with raising T.

2. The CNO cycle. The first chain releases 25,03 + (1,69) MeV, the second 24,74 + (1,98) MeV. The reactions are shown below.

$$\begin{tikzcd}
 & {}^{15}{\rm N}+{\rm p}^+\to\alpha+{}^{12}\,{\rm C} \arrow[d] & {}^{15}{\rm N}+{\rm p}^+\to\ {}^{16}{\rm O}+\gamma \arrow[d] \\
{}^{15}{\rm O}+{\rm e}^+\to\ {}^{15}{\rm N}+\overline{\nu} \arrow[ur] \arrow[urr, bend left] & {}^{12}{\rm C}+{\rm p}^+\to{}^{13}\,{\rm N}+\gamma \arrow[d] & {}^{16}{\rm O}+{\rm p}^+\to\ {}^{17}{\rm F}+\gamma \arrow[d] \\
\mathbf{{}^{14}N+p^+\to\ {}^{15}O+\boldsymbol{\gamma}} \arrow[u] & {}^{13}{\rm N}\to\ {}^{13}{\rm C}+{\rm e}^++\nu \arrow[d] & {}^{17}{\rm F}\to\ {}^{17}{\rm O}+{\rm e}^++\nu \arrow[d] \\
 & {}^{13}{\rm C}+{\rm p}^+\to{}^{14}\,{\rm N}+\gamma \arrow[ul] & {}^{17}{\rm O}+{\rm p}^+\to\alpha+{}^{14}\,{\rm N} \arrow[ull, bend left]
\end{tikzcd}$$