Theoretical Physics 3

PHYS3661

Quantum Mechanics

Epiphany 2015

Alexander Lenz

IPPP, Durham University
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Contents

Some Comments:

- 18 lectures (2 hours per week) + 3 example classes: (1 hour every 3 weeks)
  1 revision lecture in Easter
  http://www.dur.ac.uk/physics/students/problems/
  38 hours of lecture + 156 hours of preparation and reading, i.e. 4.1 hours of preparation and reading per 1 hour of lecture

- Prerequisites:

  - Foundations of Physics 2A

  - Theoretical Physics 2

  - Mathematical Methods in Physics or Analysis in many variables

  - Foundations of Physics 3A

  - Theoretical Physics 3 - Electrodynamics

- The lecture course follows the textbook:
  Quantum Mechanics; B.H. Bransden and C.J. Joachim; Prentice Hall, 2nd edition [1]
  Further recommended books for this course are Sakurai [2], Weinberg [3] (relatively advanced, from one of the masters of Quantum Field Theory), the two books from Schwabl [4, 5] (my personal favourites) and the classical book from Bjorken and Drell [6].

1 Scattering experiments and cross sections

— Chapter [13.1] of [1] —

1.1 Introduction and Motivation

The Nobel prize for physics in 2013 [8] was given to Francois Englert and Peter Higgs for the prediction (1964) of the Higgs particle [9, 10, 11, 12, 13, 14] which was discovered at the Large Hadron Collider (LHC) in 2012 [15, 16]. For more information about the discovery see www.nobelprize.org

- Press release

- Popular information

- Advanced information

The LHC - is in principle a huge microscope, which tells us about the fundamental constituents of matter.
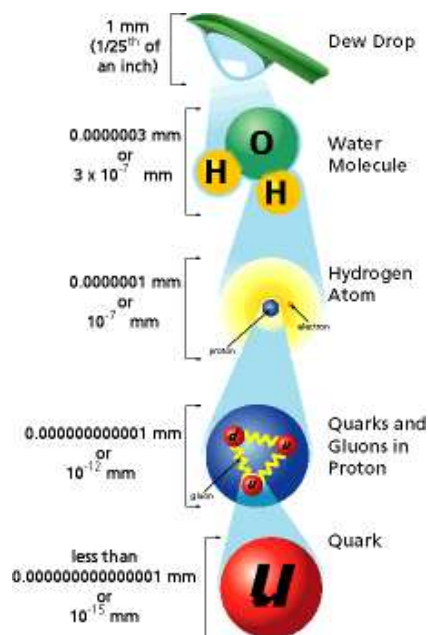
Atoms are built of electrons and the nuclei. The electrons are elementary according to the current experimental precision. The nuclei consists of nucleons, i.e. protons and neutrons. Protons and neutrons are to a first approximation built out of three quarks, which are also elementary according to the current

experimental precision.

Currently we know the following fundamental particles and forces:

- **Matter constituents**

  Quarks   Leptons

  $$\begin{pmatrix} u \\ d \end{pmatrix} \begin{pmatrix} c \\ s \end{pmatrix} \begin{pmatrix} t \\ b \end{pmatrix} \begin{pmatrix} q = +2/3 \\ q = -1/3 \end{pmatrix} \qquad \begin{pmatrix} \nu_e \\ e \end{pmatrix} \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix} \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix} \begin{pmatrix} q = 0 \\ q = -1 \end{pmatrix}$$

  - Quarks and leptons have spin $1/2$.

  - Quarks take part in all interactions, leptons do not take part in the strong interaction and neutrinos only interact via the weak interaction.

  - A proton is made out of 3 quarks: $p = |uud\rangle$

- **Fundamental forces** are carried by spin 1 (2) gauge bosons

  - Electromagnetic interaction: photon.

  - Strong interaction: 8 gluons.

  - Weak interaction: $W^{\pm}, Z$-bosons.

  - Gravity: Graviton? with spin 2.

- **Creation of mass**
  Masses of the elementary particles are in contradiction to some mathematical properties of the theory. The Higgs mechanism is a trick to solve this problem, for the price of introducing a new particle: the Higgs boson with spin 0.

This is the so-called **standard model of particle physics**, which has been experimentally verified by hundreds of experiments - sometimes with an incredible precision.

Most of this knowledge comes from scattering-experiments, like the Rutherford experiment (Geiger and Marsden 1909, Rutherford 1911) or the LHC. The corresponding scattering events take place on a microscopic level. Thus an understanding of the quantum mechanical foundations of scattering is the basis for a fundamental understanding of the building blocks of the universe.

1.2   Basics in scattering

The basic idea of scattering is simple. We have a target and some incident particles, that are flying towards and interacting with the target. In the case of Rutherford scattering the target was a gold foil and the incident particles were alpha particles (He^{++}), in the case of LHC both target and incident particles are protons.
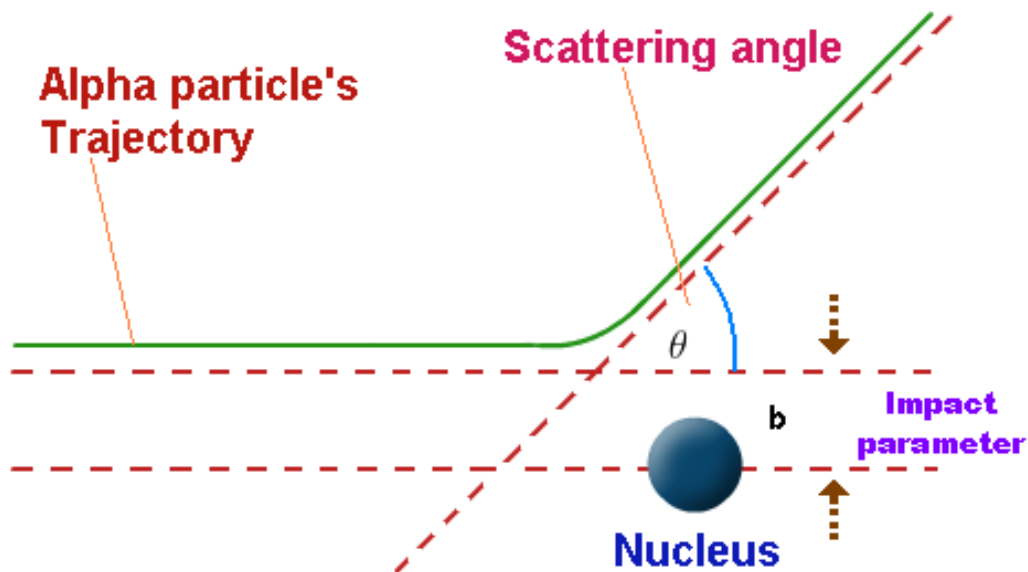
The incident particle is described by its energy E and the impact parameter b. If the incident particles and the target stay intact during the scattering process, we speak about **elastic scattering**. In that case the position of the incoming particles after scattering is given by the scattering angle (θ, ϕ) and a radial variable r.

For simplicity we assume besides elastic scattering that the target is infinitely heavy and that there is an azimuthal symmetry of the interaction.

Now we denote by $\delta\sigma$ a small area of the incoming particle flux. All particle within $\delta\sigma$ will be scattered into the solid angle element $\delta\Omega$. If we normalise the solid angle element to an unit element $d\Omega$, then the corresponding area of the incoming particles reads $d\sigma$. Having an azimuthal symmetry, the problem looks like:
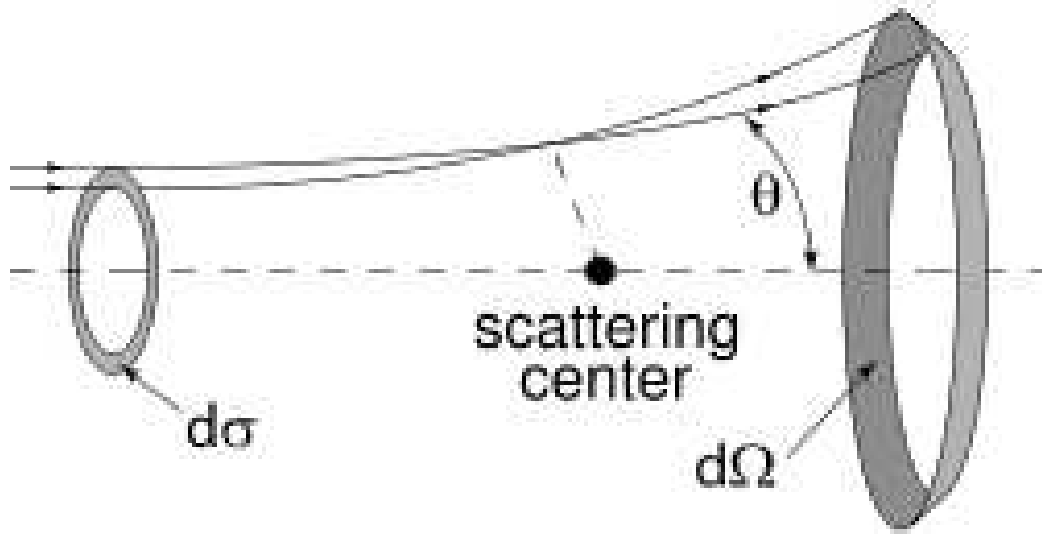
Integrating over the full solid angle $d\Omega$, will then give the effective area of the scattering target, called **total cross section** σ. Defining in addition the **differential cross-section** $d\sigma/d\Omega$ we get

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega} = \int\limits_0^{2\pi} d\phi \int\limits_0^{\pi} d\theta \sin\theta \frac{d\sigma}{d\Omega} \ . \tag{1}$$

For classical scattering of a point-like particle on a hard sphere with radius R one gets e.g.

$$\frac{d\sigma}{d\Omega} = \frac{R^2}{4} \ , \tag{2}$$

$$\sigma = \pi R^2 \ , \tag{3}$$

which coincides with our expectations above. The concept of (differential) cross sections can, however, also be applied to "soft" targets.

A beam of incoming particles can be described by the **luminosity** $\mathcal{L}$, which is defined as the number of incoming particles per unit area per time. The number of particles coming through the element $d\sigma$ per time is now called $d\dot{N}$ and we have

$$d\dot{N} = \mathcal{L} d\sigma = \mathcal{L} \frac{d\sigma}{d\Omega} d\Omega \ . \tag{4}$$

Thus the differential cross section can also be defined as

$$\frac{d\sigma}{d\Omega} := \frac{1}{\mathcal{L}} \frac{d\dot{N}}{d\Omega} \ , \tag{5}$$

which is many times used as the initial definition of the differential cross section. An elastic scattering event at LHC looks like

$$p + p \rightarrow p + p . \tag{6}$$

The total cross-section for this scattering at LHC with a proton energy of 7 TeV reads [17]

$$\sigma = (98.3 \pm 0.2(stat) \pm 2.8(syst)) \text{ mb}, \tag{7}$$

with the unit **barn** for measuring the cross section:

$$1\text{barn} = 1b = 10^{-28}m^2 = 100fm^2 . \tag{8}$$

The above concepts can also be generalised to **inelastic processes**, like the production of a Higgs particle

$$p + p \rightarrow X + H . \tag{9}$$
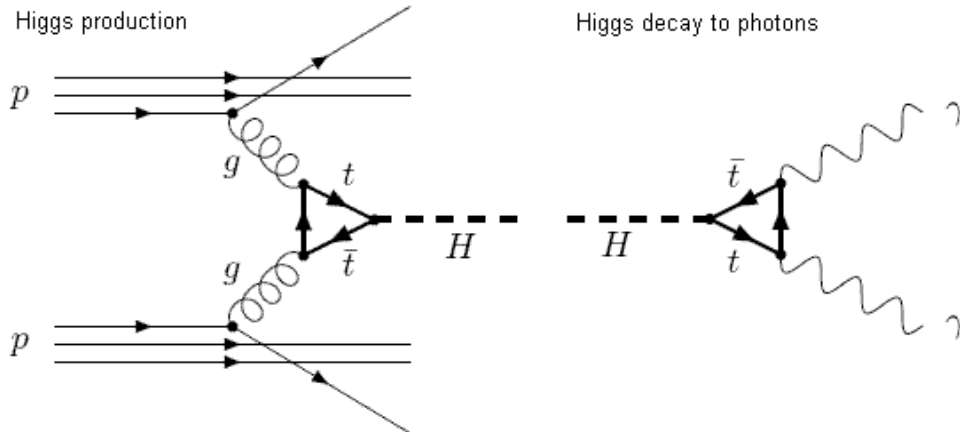
The cross section for this process is given by [19] (see e.g.[18] for a part of the state-of-the-art calculation)

$$\sigma \approx 20pb . \tag{10}$$

The number of events for an inelastic process can be determined from the **integrated luminosity**

$$\dot{N} = \mathcal{L}\sigma , \tag{11}$$

$$N = \int \mathcal{L}dt \cdot \sigma . \tag{12}$$

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The LHC achieved until now an integrated luminosity of $20(fb)^{-1}$ per experiment (ATLAS and CMS), thus the following number of Higgs particles was produced at each experiment

$$N = 20\,fb^{-1}20\,pb = 400\frac{pb}{10^{-3}pb} = 4 \cdot 10^5 \,. \tag{13}$$

To obtain the number of a certain Higgs decay like $H \to \gamma\gamma$ one has to multiply the overall number of produced Higgses with the corresponding branching ratio, in that case

$$N(H \to \gamma\gamma) = 4 \cdot 10^5 \cdot 2 \cdot 10^{-3} = 800 \,. \tag{14}$$

The value of the differential cross section for two colliding particles A and B depends on the reference frame. Two commonly used ones are the laboratory frame ($\mathbf{L}$), where particle B is in the beginning at rest and centre of mass frame ($\mathbf{CM}$). One finds

$$\tan\theta_L = \frac{\sin\theta}{\cos\theta + \tau} \,, \tag{15}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_L = \frac{(1 + \tau^2 + 2\tau\cos\theta)^{\frac{3}{2}}}{|1 + \tau\cos\theta|}\left(\frac{d\sigma}{d\Omega}\right)_{CM} \,, \tag{16}$$

with $\tau = m_A/m_B$.

- *To repeat this lecture:* Chapter [13.1] of [1]
  - the concept of cross section -

- *To prepare for next lecture:* Chapter [13.2] of [1]
  - how to calculate a cross section within quantum mechanics -

2 Potential scattering (general features)

— Chapter [13.2] of [1] —

2.1 The time-independent Schrödinger equation

Now we discuss a non-relativistic particle of mass m in a "fixed" potential, which is described by the 3-dimensional Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\Psi(\vec{r},t) \ , \tag{17}$$

where $\vec{r}$ describes the distance of the particle from the origin of the potential. *The scattering of particle A with the mass m_A with a particle B with the mass m_B due to a force that is described by the potential is given by*

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V(\vec{r})\right]\Psi(\vec{r},t) \ , \tag{18}$$

where μ is the reduced mass and $\vec{r} = \vec{r}_A - \vec{r}_B$ is the relative distance between the two particles. This is e.g. the case at LHC, where two protons scatter, but with relativistic energies. But here we concentrate first on the fixed potential case.

If the potential does not depend on time - as in our case - we can separate the time dependence and we look for **stationary solutions**:

$$\Psi(\vec{r},t) =: \Psi(\vec{r})e^{-i\frac{E}{\hbar}t} \ . \tag{19}$$

The wave function $\Psi(\vec{r})$ has to satisfy the time-independent Schrödinger-equation

$$E\Psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\Psi(\vec{r}) \ , \tag{20}$$

where the energy E of the particle can be written as

$$E =: \frac{\vec{p}^2}{2m} =: \frac{\hbar^2\vec{k}^2}{2m} =: \frac{1}{2}m\vec{v}^2 \ , \tag{21}$$

with

- the incident momentum of the particle $\vec{p} = \hbar\vec{k} = m\vec{v}$,

- the incident wave vector of the particle $\vec{k}$,

- the incident velocity of the particle $\vec{v}$.

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Now we can rewrite Eq.(20) as

$$\boxed{\left[\vec{\nabla}^2 + \vec{k}^2 - U(\vec{r})\right]\Psi(\vec{r}) = 0 \,,} \tag{22}$$

with the redefined potential

$$U(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r})\,. \tag{23}$$

We will devote now several lectures to different solutions of Eq.(22)

2.2 The scattering amplitude

Now we derive a formula that directly relates the solution of the Schrödinger equation to a measurable cross section. In this subsection we do this by making several rough approximations in order to get fast to the desired result. Later on in this lecture course we will directly derive the formula.

For large distances $\vec{r}$ we split up the wave function in an incoming part and a scattered part

$$\Psi(\vec{r}) \xrightarrow[r \to \infty]{} \Psi_{inc.}(\vec{r}) + \Psi_{scat.}(\vec{r})\,. \tag{24}$$

For large distances we typically can neglect the potential term in Eq.(22) and we get the free equation

$$\left[\vec{\nabla}^2 + \vec{k}^2\right]\Psi(\vec{r}) = 0 \,, \tag{25}$$

Now we describe the incoming particle with a plane wave, i.e. all the incoming particles have the same momentum $\vec{p} = \hbar\vec{k}$ and travel all in the same direction, which choose to be the z-direction.

$$\Psi_{inc.}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = e^{ikz}\,. \tag{26}$$

This fulfils Eq.(25). With this normalisation we have for the particle density $\rho = |\Psi_{inc.}(\vec{r})|^2 = 1$, i.e. one particle per unit volume. Thus the incident flux reads

$$F = v \cdot \rho = \frac{p}{m}\rho\,, \tag{27}$$

$$\left[\frac{1}{m^2 s}\right] = \left[\frac{m}{s} \cdot \frac{1}{m^3}\right]\,. \tag{28}$$

The outgoing particle we want to describe by an outgoing wave

$$\Psi_{scat.}(\vec{r}) = f(k, \theta, \phi)\frac{e^{ikr}}{r}\,, \tag{29}$$

with the **scattering amplitude** $f(k, \theta, \phi)$. The factor $1/r$ is needed for the conservation of probability. This wave function also fulfils Eq.(25) for very large values of r.

Thus we get for the full asymptotic wave function:

$$\psi_{\vec{k}} \xrightarrow[r \to \infty]{} e^{i\vec{k} \cdot \vec{r}} + f(k, \theta, \phi) \frac{e^{ikr}}{r} \ . \tag{30}$$

This ansatz can now be used to calculate the current density $\vec{j}$

$$\vec{j}(\vec{r}) = \frac{\hbar}{2mi} \left[\Psi^*(\vec{\nabla}\Psi) - (\vec{\nabla}\Psi^*)\Psi \right] \tag{31}$$

and one gets

$$j_r = \frac{\hbar k}{m} \frac{|f(k, \theta, \phi)|^2}{r^2} \ . \tag{32}$$

j_r represents the number of particles crossing a unit area per unit time and the detector presents a cross-sectional area $r^2 d\Omega$ to the scattered beam. The number of particles entering the detector per unit time, $d\dot{N}$ is

$$
\begin{aligned}
d\dot{N} &= j_r r^2 d\Omega = \frac{\hbar k}{m} |f(k, \theta, \phi)|^2 \, d\Omega && (33) \\
&= v \, |f(k, \theta, \phi)|^2 \, d\Omega && (34) \\
&= \frac{F}{\rho} \, |f(k, \theta, \phi)|^2 \, d\Omega \ . && (35)
\end{aligned}
$$

$d\dot{N}$ can also be described by the incoming flux F and the area $d\sigma$ these particles are crossing before the scattering:

$$d\dot{N} = F d\sigma = F \frac{d\sigma}{d\Omega} d\Omega \ . \tag{36}$$

Equating the two expressions and using $\rho = 1$ we get our master formula

$$\boxed{\frac{d\sigma}{d\Omega} = |f(k, \theta, \phi)|^2 \ .} \tag{37}$$

The differential cross section is measured in the experiment, while the scattering amplitude is calculated in theory, by solving the Schrödinger equation.

- *To repeat this lecture:* Chapter [13.2] of [1]

- *To prepare for next lecture:* Chapter [7.3/4] of [1]

3   Spherical Bessel functions

Before continuing with the scattering problems we make some mathematics
interlude and introduce special functions that will be very helpful for the
solution of the Schr¨ödinger equation.

3.1   Separation of variables

This time we consider a spherical symmetric potential, i.e.

$$V(\vec{r}) = V(r = |\vec{r}|) \ . \tag{38}$$

To proceed we rewrite the Laplace operator in spherical coordinates

$$\vec{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{39}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\vec{L}^2}{\hbar^2 r^2} \ , \tag{40}$$

with the angular momentum operator $\vec{L}$. Next we separate the radial and
the angular dependence of the solution

$$\Psi(\vec{r}) = \sum_{E,l,m} c_{Elm}\Psi_{Elm}(\vec{r}) \tag{41}$$

$$\Psi_{Elm}(\vec{r}) = R_{El}(r)Y_{lm}(\theta,\phi) \ , \tag{42}$$

with the radial function R_{El} that has to be determined and the well-known
spherical harmonics Y_{lm} (TP2, Edynamics).
The spherical harmonics can be expressed in terms of **associated Legendre
functions** *and these in terms of* **Legendre polynomials** *- see also the
corresponding Wikipedia articles.*

$$Y_{lm}(\theta,\phi) = C_{lm}e^{im\phi}P_l^m(\cos\theta) \ , \tag{43}$$

$$P_l^m(x) = (1-x^2)^{\frac{|m|}{2}}\left(\frac{d}{dx}\right)^{|m|}P_l(x) \ , \tag{44}$$

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l \ . \tag{45}$$

The following orthogonality relations hold

$$\int Y_l^m Y_{l'}^{m'*} d\Omega = \delta_{ll'}\delta_{mm'} , \qquad (46)$$

$$\int_{-1}^{1} P_k^m(x)P_l^k(x)dx = \frac{2(l+m)!}{(2l+1)(l-m)!}\delta_{ml} , \qquad (47)$$

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \frac{2}{2n+1}\delta_{mn} . \qquad (48)$$

Having a cylinder symmetry the solutions will be even more simple and there is no dependence on m, which can then be set to 0 and thus the spherical functions are simply replaced by Legendre polynomials:

$$Y_{lm}(\theta,\phi) \rightarrow P_l(\cos\theta) . \qquad (49)$$

Coming back to the general case and using

$$\vec{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi) , \qquad (50)$$

we get for the time-independent Schrödinger equation in Eq.(22)

$$\left[\vec{\nabla}^2 - U(r) + \vec{k}^2\right]\Psi_{Elm}(\vec{r}) = 0 \qquad (51)$$

$$\left\{\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\vec{L}^2}{\hbar^2 r^2}\right] - U(r) + \vec{k}^2\right\}R_{El}(r)Y_{lm}(\theta,\phi) = 0 \qquad (52)$$

$$\left\{\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2}\right] - U(r) + \vec{k}^2\right\}R_{El}(r) = 0 \qquad (53)$$

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} - U(r) + \vec{k}^2\right]R_{El}(r) = 0 . \qquad (54)$$

Eq.(54) is now the defining equation for the radial part of the Schrödinger equation - the only missing part.

3.2 The simplest Bessel function

To get an idea how the solutions of Eq.(54) might look like, we start by considering the free particle case, i.e. $U(r) = 0$. Defining $u_{El}(r) := rR_{El}(r)$ we are left with

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + \vec{k}^2\right]\frac{u_{El}(r)}{r} = 0 \qquad (55)$$

$$\left[\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} + \vec{k}^2\right]u_{El}(r) = 0 . \qquad (56)$$

Taking in addition $l = 0$ we get

$$\left[\frac{\partial^2}{\partial r^2} + \vec{k}^2\right] u_{E0}(r) = 0 , \qquad (57)$$

which is solved by

$$u_{E0}(r) = A \sin(kr) + B \cos(kr) . \qquad (58)$$

Thus we finally get

$$R_{E0} = A \frac{\sin(kr)}{r} + B \frac{\cos(kr)}{r} . \qquad (59)$$

The cosine part gives a divergent function R_{El}, at the origin, to avoid that one simply can set $B = 0$.

3.3 The spherical Bessel equation

3.3.1 Definition

To solve Eq.(55) for general values of l we stay with the notion of the radial function R_{El} and make a change of variables to $\rho := kr$ to get

$$\boxed{\left[\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2} + 1\right] R_l(\rho) = 0 ,} \qquad (60)$$

where we denoted $R_l(\rho) := R_{El}(\rho/k)$. Eq.(60) is called the **spherical Bessel differential equation**. We know the solution for $l = 0$ already

$$R_0(\rho) = Ak \frac{\sin(\rho)}{\rho} + Bk \frac{\cos(\rho)}{\rho} . \qquad (61)$$

3.3.2 Deriving the solution:

Now we either look into some Mathbook or we use some tricks:

- Trick 1: For $l \neq 0$ we make the Ansatz $R_l(\rho) =: \rho^l \chi_l(\rho)$ and Eq.(60) turns into
$$\left[\frac{\partial^2}{\partial \rho^2} + \frac{2(l+1)}{\rho} \frac{\partial}{\partial \rho} + 1\right] \chi_l(\rho) = 0 . \qquad (62)$$

- Trick 2: Next we try to derive a recursion relation.

  – Assume that $\chi_l(\rho)$ is a solution of Eq.(62).

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– What equation holds for[1]

$$\chi(\rho) := \frac{1}{\rho} \frac{\partial \chi_l(\rho)}{\partial \rho} \ ? \tag{63}$$

To answer that we differentiate Eq.(62) once more

$$\left[\frac{\partial^3}{\partial \rho^3} + \frac{2(l+1)}{\rho} \frac{\partial^2}{\partial \rho^2} - \frac{2(l+1)}{\rho^2} \frac{\partial}{\partial \rho} + \frac{\partial}{\partial \rho} \right] \chi_l(\rho) = 0 \tag{64}$$

$$\left[\frac{\partial^2}{\partial \rho^2} + \frac{2(l+1)}{\rho} \frac{\partial}{\partial \rho} - \frac{2(l+1)}{\rho^2} + 1 \right] (\rho \chi(\rho)) = 0 \tag{65}$$

$$\left[\frac{\partial^2}{\partial \rho^2} + \frac{2(l+2)}{\rho} \frac{\partial}{\partial \rho} + 1 \right] \chi(\rho) = 0 \ . \tag{66}$$

The last line is simply the defining equation for $\chi_{l+1}(\rho)$. Thus we have the desired recursion relation

$$\chi_{l+1}(\rho) = \frac{1}{\rho} \frac{\partial \chi_l(\rho)}{\partial \rho} \tag{67}$$

leading to

$$\chi_l(\rho) = \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l \chi_0(\rho) \ . \tag{68}$$

With $\chi_0(\rho)$ given in Eq.(59) we get two fundamental solutions of Eq.(60): the **spherical Bessel functions** (or **Spherical Bessel functions of the first kind**) $j_l(\rho)$ and the **spherical Neumann functions** (or **spherical Bessel functions of the second kind**) $n_l(\rho)$.[2]

$$R_l(\rho) = j_l(\rho) := (-1)^l \rho^l \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l \frac{\sin \rho}{\rho} \ , \tag{69}$$

$$R_l(\rho) = n_l(\rho) := -(-1)^l \rho^l \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \right)^l \frac{\cos \rho}{\rho} \ . \tag{70}$$

The factors $\pm(-1)^l$ are just convention.

Eq.(55) is then solved by $R_{El}(r) = j_l(kr)$ and $R_{El}(r) = n_l(kr)$.

---

[1]Clearly, quite some trial and error was necessary to get this idea!

[2]The MATHEMATICA notation reads $j_l(x) = SphericalBesselJ[l, x]$ and $n_l(x) = SphericalBesselY[l, x]$.

3.3.3 Properties of the solutions

The first few functions read

$$
j_0(\rho) = \frac{\sin \rho}{\rho} \tag{71}
$$

$$
j_1(\rho) = \frac{\sin \rho}{\rho^2} - \frac{\cos \rho}{\rho} \tag{72}
$$

$$
j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho} \right) \sin \rho - \frac{3}{\rho^2} \cos \rho \tag{73}
$$

and

$$
n_0(\rho) = -\frac{\cos \rho}{\rho} \tag{74}
$$

$$
n_1(\rho) = -\frac{\cos \rho}{\rho^2} - \frac{\sin \rho}{\rho} \tag{75}
$$

$$
n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho} \right) \cos \rho - \frac{3}{\rho^2} \sin \rho \tag{76}
$$

Spherical Bessel functions $j_0(x), j_1(x)$ and $j_2(x)$
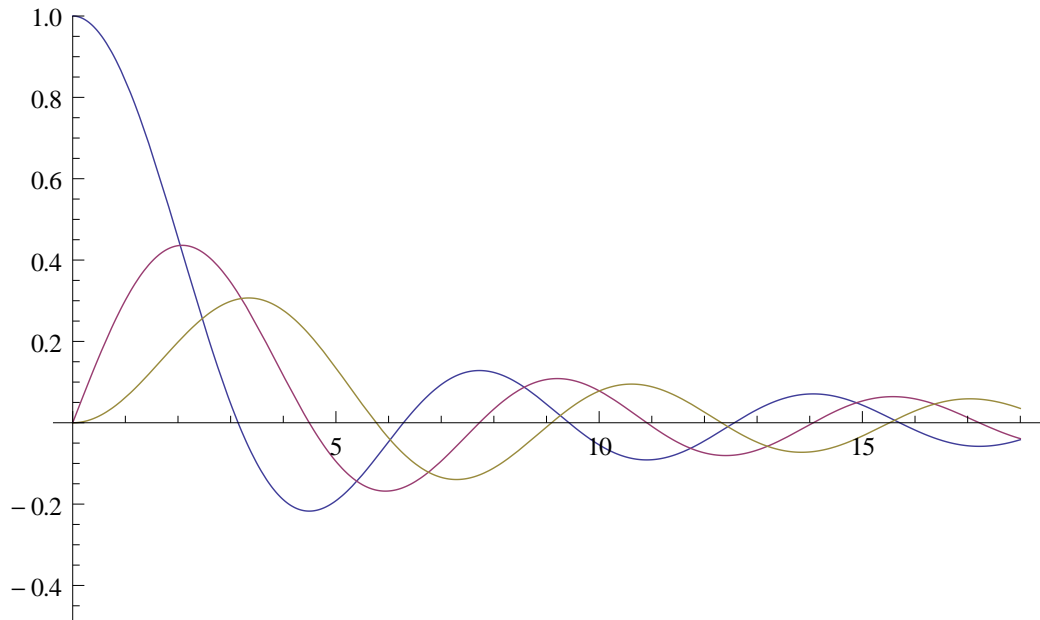
Spherical Neumann functions $n_0(x), n_1(x)$ and $n_2(x)$
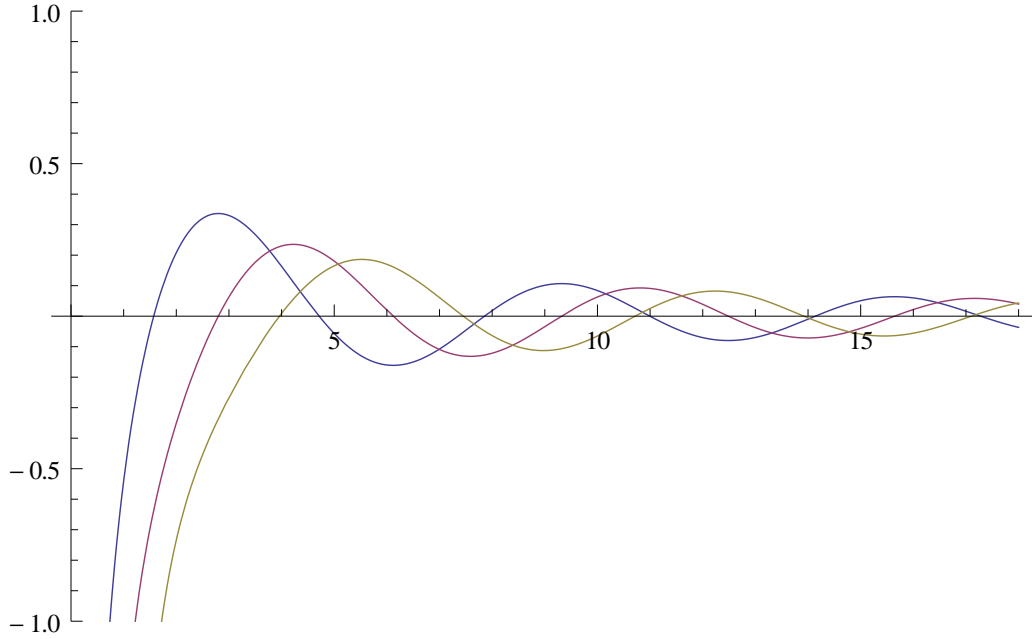
For small values of ρ these functions can be expanded as

$$j_l(\rho) \approx \frac{2^l l!}{(2l+1)!} \rho^l \, , \tag{77}$$

$$n_l(\rho) \approx . \frac{(2l)!}{2^l l!} \rho^{-(l+1)} \, . \tag{78}$$

For large values of ρ the functions can be approximated by

$$j_l(\rho) \approx \frac{1}{\rho} \sin\left(\rho - \frac{l\pi}{2}\right) \, , \tag{79}$$

$$n_l(\rho) \approx -\frac{1}{\rho} \cos\left(\rho - \frac{l\pi}{2}\right) \, . \tag{80}$$

3.3.4 Bessel functions J_ν

The spherical Bessel functions $j_l(\rho)$ and the spherical Neumann functions $n_l(\rho)$, that can both be expressed in terms of **ordinary Bessel functions** $J_\nu(\rho)$ of order ν.

$$j_l(\rho) = \left(\frac{\pi}{2\rho}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(\rho) \tag{81}$$

$$n_l(\rho) = (-1)^{l+1} \left(\frac{\pi}{2\rho}\right)^{\frac{1}{2}} J_{-l-\frac{1}{2}}(\rho) \tag{82}$$

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3.3.5 Spherical Hankel functions $h_\nu^{(1,2)}$

These functions are just linear combinations of the spherical Bessel and Neumann functions

$$
\begin{align}
h_\nu^{(1)}(\rho) &= j_\nu(\rho) + i n_\nu(\rho) \tag{83} \\
h_\nu^{(2)}(\rho) &= j_\nu(\rho) - i n_\nu(\rho) = \left[h_\nu^{(1)}(\rho) \right]^* \tag{84}
\end{align}
$$

3.3.6 Orthogonality relations

3.4 Summary of Bessel functions

Taking a vanishing potential in Eq.(54) we get

$$
\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + \vec{k}^2 \right] R_{El}(r) = 0 . \tag{85}
$$

This equation is solved by

$$
R_{El}(r) = A j_l(kr) + B n_l(kr) . \tag{86}
$$

Thus the whole 3-dimensional Schrödinger equation is solved by

$$
\Psi(\vec{r}) = \sum_{E,l,m} c_{ELM} \left[A j_l(kr) + B n_l(kr) \right] Y_{lm}(\theta, \phi) . \tag{87}
$$

This means that spherical harmonics in combination with spherical Bessel functions form a complete set of solutions for the free 3-dimensional Schrödinger equation.

3.5 Plane waves

Plane waves are a different complete set of solutions for the free 3-dimensional Schrödinger equation. Hence there is transformation between plane waves and spherical harmonics in combination with spherical Bessel functions.
We give here the expression of a plane wave in term of spherical Bessel functions and Legendre polynomials or spherical harmonics without derivation

$$
\begin{align}
e^{i\vec{k}\vec{r}} &= \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) \tag{88} \\
&= 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\vec{k}) Y_{lm}(\vec{r}) . \tag{89}
\end{align}
$$

- *To repeat this lecture:* Chapter [7.3/4] of [1]

- *To prepare for next lecture:* Chapter [13.3/4] of [1]

4 The method of partial waves

4.1 Definition of partial waves

After our mathematics excursion we turn back to the ansatz for the general scattering solution, given in Eq.(30).

$$\psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}} + f(k,\theta,\phi)\frac{e^{ikr}}{r} \ . \tag{90}$$

If we have a central potential $V = V(r)$, we have an azimuthal symmetry, i.e. there is no dependence on the angle ϕ. We choose the z-axis such, that the incoming particles fly along this axis. In that case the full wave function $\psi_{\vec{k}}$ and the scattering amplitude $f(k,\theta)$ can be expanded in terms of Legendre polynomials

$$\psi_{\vec{k}} = \sum_{l=0}^{\infty} R_l(k,r)P_l(\cos\theta) \ , \tag{91}$$

$$f(k,\theta) = \sum_{l=0}^{\infty} f_l(k)P_l(\cos\theta) \ . \tag{92}$$

Each term in the sum in Eq.(91) is called a **partial wave** and it is simultaneously an eigenfunction of $\vec{L}^2$ and L_z with eigenvalues $l(l+1)\hbar^2$ and 0. Using the spectroscopic notation we denote the $l = 0, 1, 2, 3, ,..$ wave by $s, p, d, f, ...$ wave.

The coefficients $f_l(k)$ in the expansion of the scattering amplitude are called **partial wave amplitudes**. According to our master formula for the cross

section, we get

$$\frac{d\sigma}{d\Omega} = |f(k,\theta)|^2 \tag{93}$$

$$= \sum_{l'=0}^{\infty} \sum_{l=0}^{\infty} f_{l'}^*(k) f_l(k) P_{l'}(\cos\theta) P_l(\cos\theta) \ . \tag{94}$$

$$\Rightarrow \sigma = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_{-1}^{+1} \frac{d\sigma}{d\Omega} d\cos\theta \tag{95}$$

$$= 2\pi \sum_{l'=0}^{\infty} \sum_{l=0}^{\infty} f_{l'}^*(k) f_l(k) \int_{-1}^{+1} P_{l'}(x) P_l(x) dx \tag{96}$$

$$= 4\pi \sum_{l=0}^{\infty} \frac{1}{2l+1} |f_l(k)|^2 = \sum_{l=0}^{\infty} \sigma_l \ . \tag{97}$$

Thus a knowledge of the partial wave amplitudes gives immediately the total cross section. The relation between the partial wave amplitudes and the radial function $R_l(k,r)$ in the partial wave can be derived as follows:

$$\psi_{\vec{k}} = e^{i\vec{k}\cdot\vec{r}} + f(k,\theta,\phi) \frac{e^{ikr}}{r} \tag{98}$$

$$\sum_{l=0}^{\infty} R_l(k,r) P_l(\cos\theta) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) + \sum_{l=0}^{\infty} f_l(k) P_l(\cos\theta) \frac{e^{ikr}}{r} \tag{99}$$

$$\Rightarrow R_l(k,r) = (2l+1) i^l j_l(kr) + f_l(k) \frac{e^{ikr}}{r} \tag{100}$$

4.2 Structure of the solution - Phase shifts

Next we investigate a little more the general structure of the solution of the radial equation $R_l(k,r)$.

For large values of $r > d$ we neglect the contribution of the potential and get as a general solution

$$R_l(k,r) = B_l(k) j_l(kr) + C_l(k) n_l(kr) \ . \tag{101}$$

The coefficients B_l and C_l will be determined by matching with the region $r < d$, where the effects of the potential have to be taken into account. For very large values of r we can use the asymptotic expression for the spherical

Bessel and Neumann functions

$$R_l(k,r) = \frac{1}{kr} \left[B_l(k) \sin \left(kr - \frac{l\pi}{2} \right) - C_l(k) \cos \left(kr - \frac{l\pi}{2} \right) \right] . \qquad (102)$$

By defining

$$A_l(k) \; := \; \sqrt{B_l(k)^2 + C_l(k)^2} , \qquad (103)$$

$$\tan \delta_l(k) \; := \; -\frac{C_l(k)}{B_l(k)} \; , \sin \delta_l(k) := -\frac{C_l(k)}{A_l(k)} \; , \cos \delta_l(k) := \frac{B_l(k)}{A_l(k)} \; , (104)$$

we get

$$R_l(k,r) \; = \; \frac{A_l(k)}{kr} \left[\cos \delta_l(k) \sin \left(kr - \frac{l\pi}{2} \right) + \sin \delta_l(k) \cos \left(kr - \frac{l\pi}{2} \right) \right] \qquad (105)$$

$$= \; \frac{A_l(k)}{kr} \sin \left(kr - \frac{l\pi}{2} + \delta_l(k) \right) . \qquad (106)$$

The $\delta_l(k)$ are called **phase shifts** and they denote the strength of the scattering in the l-th partial wave.

If there is no potential at all acting, then the solution in Eq.(102) has to hold everywhere and in particular for $r = 0$. Since $n_l(r)$ is singular at $r = 0$, the corresponding coefficient has to be set to 0, $C_l(k) = 0$. In that case we get also a vanishing phase shift $\delta_l(k) = 0$.

Combing the asymptotic form of the radial function with our result from Eq.(100) we get

$$\frac{A_l(k)}{kr} \sin \left(kr - \frac{l\pi}{2} + \delta_l(k) \right) \; = \; (2l+1)i^l \frac{\sin \left(kr - \frac{l\pi}{2} \right)}{kr} + f_l(k) \frac{e^{ikr}}{r} , \qquad (107)$$

which can be solved by

$$A_l(k) \; = \; (2l+1)i^l e^{i\delta_l(k)} , \qquad (108)$$

$$f_l(k) \; = \; \frac{2l+1}{2ik} \left[e^{2i\delta_l(k)} - 1 \right] . \qquad (109)$$

With this we get some final expressions for the scattering amplitude and for the differential cross section:

$$f(k,\theta) \; = \; \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left[e^{2i\delta_l(k)} - 1 \right] P_l(\cos \theta) , \qquad (110)$$

$$\sigma_l \; = \; \frac{4\pi}{2l+1} |f_l(k)|^2 , \qquad (111)$$

$$= \; \frac{4\pi(2l+1)}{k^2} \sin^2 \delta_l(k) . \qquad (112)$$

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Therefore the knowledge of the scattering phase is sufficient to solve a scattering problem.

Setting $\theta = 0$ in Eq.(110) we get

$$\Im\left[f(k,0)\right] = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\Im\left[e^{i\delta_l(k)}\frac{e^{i\delta_l(k)} - e^{-i\delta_l(k)}}{2i}\right] \qquad (113)$$

$$= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k) \qquad (114)$$

$$= \frac{k}{4\pi}\sigma \ . \qquad (115)$$

This is the famous **Optical Theorem**: the total cross section is given by the forward ($\theta = 0$) scattering amplitude.

4.3 Convergence of the partial wave expansion

- For large values of l the term $l(l+1)/r^2$ will dominate over the potential $U(r)$ thus the latter one can be neglected and the solution is equal to the free solution, having no phase shift and thus no contribution to the cross section.

- An estimate gives that values of $l > ka$ can be neglected, if a being the extension of the potential.

- For $k \to 0$ only $l = 0$ contributes (**s-wave scattering**). Defining the **scattering length** l_s as

$$l_s := -\lim_{k \to 0}\frac{\tan\delta_0(k)}{k} \ , \qquad (116)$$

one finds

$$f \xrightarrow[k \to 0]{} -l_s \ , \qquad (117)$$

$$\frac{d\sigma}{d\Omega} \xrightarrow[k \to 0]{} l_s^2 \ , \qquad (118)$$

$$\sigma \xrightarrow[k \to 0]{} 4\pi l_s^2 \ . \qquad (119)$$

4.4 Scattering by a square well

—-

4.5 Resonances

According to Eq.(112) the l-th partial cross section reads

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\frac{1}{1+\cot^2\delta_l(k)} \ . \qquad (120)$$

The energy where $\cot\delta_l(k)$ becomes zero is called **resonance energy** E_R. At the resonance one can write

$$\cot\delta_l(k) = \frac{E_R - E}{\Gamma(E_R)/2} \ , \qquad (121)$$

with the **resonance width** $\Gamma(E_R)$. This leads to the **Breit-Wigner resonance formula**

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2(E_R)/4}{(E-E_R)^2 + \Gamma^2(E_R)/4} \ , \qquad (122)$$

which is valid in the vicinity of a resonance. For $M \equiv E_R$ it looks like:
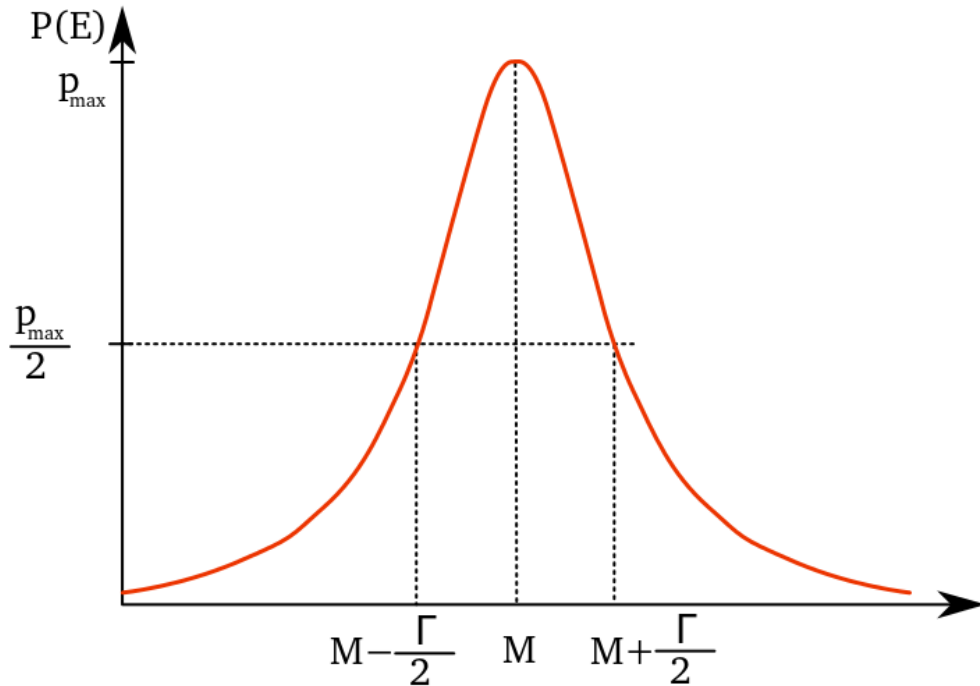
In practice the resonances are typically superimposed by background scattering, e.g. from other partial waves. Here we show an example for resonances found at the LHC, when looking for the dimuon final state in proton scattering: $p + p \rightarrow \mu^+ + \mu^-$.
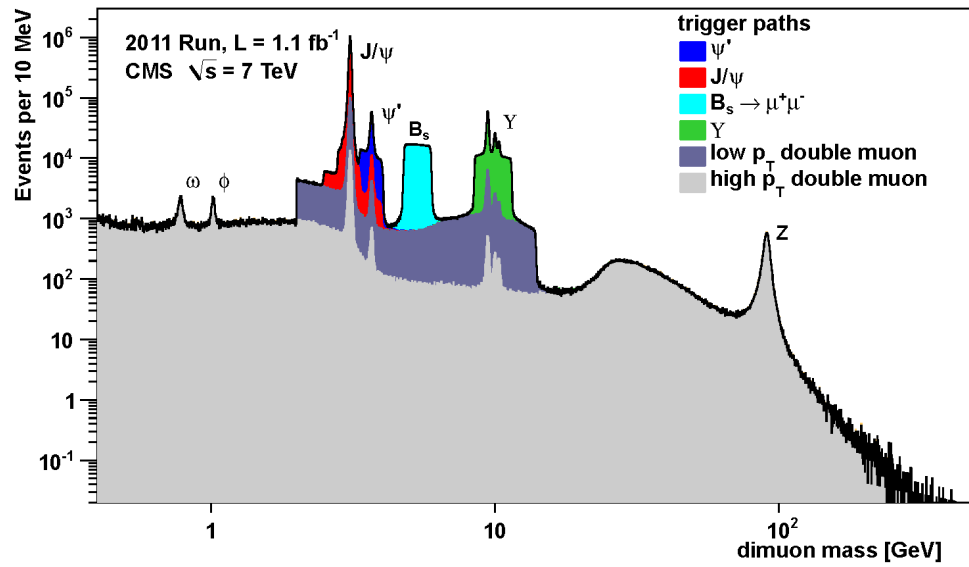
4.6 Hard-sphere potential

- *To repeat this lecture:* Chapter [13.3/4] of [1]

- *To prepare for next lecture:* Chapter [13.5] of [1]

5 The integral equation of potential scattering

— Chapter [13.5] of [1] —

In this lecture we start considering non-trivial potentials and we will re-express Eq.(22) by an integral equation.

5.1 Definition of the Green's function

Eq.(22) can be written as

$$\boxed{\left[\vec{\nabla}^2 + \vec{k}^2\right]\Psi(\vec{r}) = U(\vec{r})\Psi(\vec{r}) \ .} \tag{123}$$

The general solution of this equation can be expressed as

$$\Psi(\vec{r}) = \Psi_0(\vec{r}) + \int G_0(k, \vec{r} - \vec{r}')U(\vec{r}')\Psi(\vec{r}')d\vec{r}' \ , \tag{124}$$

with $\Psi_0(\vec{r})$ being a solution of the homogeneous Schrödinger equation

$$\left[\vec{\nabla}^2 + \vec{k}^2\right]\Psi_0(\vec{r}) = 0 \tag{125}$$

and the **Green's function** $G_0(k, \vec{r} - \vec{r}')$, which is defined as

$$\left[\vec{\nabla}^2 + \vec{k}^2\right]G_0(k, \vec{r} - \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}') \ . \tag{126}$$

If we choose the homogeneous solution to be a plane wave, we get

$$\Psi_{0,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \ , \tag{127}$$

$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int G_0(k, \vec{r} - \vec{r}')U(\vec{r}')\Psi_{\vec{k}}(\vec{r}')d\vec{r}' \ . \tag{128}$$

5.2 Deriving the Green's function

In order to derive the Green's function, we consider the Fourier transformation of the definition of the Green's function, Eq.(126).

$$G_0(k, \vec{r}) = \int \frac{d^3q}{(2\pi)^3}\tilde{G}_0(k, \vec{q})e^{i\vec{q}\cdot\vec{r}} \ , \tag{129}$$

$$\left(\Delta + k^2\right)G_0(k, \vec{r}) = \int \frac{d^3q}{(2\pi)^3}(k^2 - q^2)\tilde{G}_0(k, \vec{q})e^{i\vec{q}\cdot\vec{r}} \overset{!}{=} \delta^{(3)}(\vec{r}) = \int \frac{d^3q}{(2\pi)^3}e^{i\vec{q}\cdot\vec{r}} \ , \tag{130}$$

$$\Rightarrow \tilde{G}_0(k, \vec{q}) = \frac{1}{k^2 - q^2} \ . \tag{131}$$

Now we have a solution for the Fourier transform of the Green's function, so we are left with transforming $\tilde{G}_0(k, \vec{q})$ back to $G_0(k, \vec{r})$.

$$G_0(k, \vec{r}) \quad = \quad \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\vec{q}\cdot\vec{r}}}{k^2 - q^2} \tag{132}$$

$$\overset{Angular\ integr.}{=} \quad -\frac{1}{4\pi^2 ir} \int\limits_{-\infty}^{\infty} \frac{qe^{iqr}}{q^2 - k^2} dq \tag{133}$$

$$\overset{PFD}{=} \quad -\frac{1}{4\pi r} \frac{1}{2\pi i} \int\limits_{-\infty}^{\infty} \left(\frac{e^{iqr}}{q+k} + \frac{e^{iqr}}{q-k} \right) dq \tag{134}$$

$$\overset{Cauchy}{=} \quad -\frac{e^{ikr}}{4\pi r} \ . \tag{135}$$

This is the final result for the Green's function!

5.3 Lippmann-Schwinger equation

Thus the general solution of Eq.(22) reads

$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}')\Psi_{\vec{k}}(\vec{r}')d\vec{r}' \ . \tag{136}$$

This integral equation is called the **Lippmann-Schwinger equation**.
For a potential with a finite extension, i.e. $U(r) = 0$ for $r > d$, we can investigate the limit $r \to \infty$ and $r' < d \ll r$ to get

$$|\vec{r}-\vec{r}'| \quad \to \quad r - \frac{\vec{r}}{r}\cdot\vec{r}' + ... \ , \tag{137}$$

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \quad \to \quad \frac{e^{ikr}}{r}e^{-i\vec{k}'\cdot\vec{r}'} + ... \ , \tag{138}$$

with $\vec{k}' = \vec{r}/r\ k$. This leads to

$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r}f(k, \theta, \phi) \ , \tag{139}$$

with

$$f(k, \theta, \phi) \quad = \quad -\frac{1}{4\pi} \int e^{-i\vec{k}'\cdot\vec{r}'} U(\vec{r}')\Psi_{\vec{k}}(\vec{r}')d\vec{r}'$$

$$= \quad -\frac{1}{4\pi} \langle \Psi_{0,\vec{k}}|U|\Psi_{\vec{k}}\rangle \ . \tag{140}$$

Remarks:

- This is now the promised derivation of Eq.(30).

- The **transition matrix element** $T_{\vec{k}'\vec{k}}$ is defined as

$$T_{\vec{k}'\vec{k}} := \langle \Psi_{0,\vec{k}} | V | \Psi_{\vec{k}} \rangle \ . \tag{141}$$

- The differential cross section can be expressed as

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2 \hbar^4} \left| T_{\vec{k}'\vec{k}} \right|^2 \ . \tag{142}$$

- *To repeat this lecture:* Chapter [13.5] of [1]

- *To prepare for next lecture:* Chapter [13.6] of [1]

6 The Born approximation

In this lecture we finally derive an approximation for the solution of the general scattering problem.

6.1 The Born series

Eq.(128) can be also written as

$$\Psi_{\vec{k}}(\vec{r}') \;=\; e^{i\vec{k}\cdot\vec{r}'} + \int G_0(k,\vec{r}'-\vec{r}'')U(\vec{r}'')\Psi_{\vec{k}}(\vec{r}'')d\vec{r}'' \,. \qquad (143)$$

Inserting Eq.(143) into Eq.(128) gives

$$\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int G_0(k,\vec{r}-\vec{r}')U(\vec{r}')\left[e^{i\vec{k}\cdot\vec{r}'} + \int G_0(k,\vec{r}'-\vec{r}'')U(\vec{r}'')\Psi_{\vec{k}}(\vec{r}'')d\vec{r}''\right]d\vec{r}' \,.$$
$$(144)$$

In the next step we replace $\Psi_{\vec{k}}(\vec{r}'')$ by the whole integral solution and so on. In the end we get an expansion like

$$\Psi_0(\vec{r}) \;=\; e^{i\vec{k}\cdot\vec{r}}\,, \qquad\qquad\qquad\qquad\qquad (145)$$

$$\Psi_1(\vec{r}) \;=\; e^{i\vec{k}\cdot\vec{r}} + \int G_0(k,\vec{r}-\vec{r}')U(\vec{r}')e^{i\vec{k}\cdot\vec{r}'}d\vec{r}' \,, \qquad (146)$$

$$\Psi_2(\vec{r}) \;=\; e^{i\vec{k}\cdot\vec{r}} + \int G_0(k,\vec{r}-\vec{r}')U(\vec{r}')e^{i\vec{k}\cdot\vec{r}'}d\vec{r}'$$
$$+ \int G_0(k,\vec{r}-\vec{r}')U(\vec{r}')\int G_0(k,\vec{r}'-\vec{r}'')U(\vec{r}'')e^{i\vec{k}\cdot\vec{r}''}d\vec{r}''d\vec{r}' \,(147)$$
$$... \;=\; ...$$

If the potential U gives rise to a small perturbation of the system, then such an expansion might converge and the real result could be approximated by the first terms.

6.2 The first Born approximation

We get for the first Born approximation of the scattering amplitude

$$f^B(k,\theta,\phi) \;=\; -\frac{1}{4\pi}\int e^{-i\vec{k}'\cdot\vec{r}}U(\vec{r})e^{i\vec{k}\cdot\vec{r}}d\vec{r} \qquad (148)$$

$$=\; -\frac{1}{4\pi}\int e^{i\vec{\Delta}\cdot\vec{r}}U(\vec{r})d\vec{r}\,, \qquad (149)$$

with the **momentum transfer** $\hbar\vec{\Delta}$.

$$\vec{\Delta} := \vec{k} - \vec{k}' . \tag{150}$$

Thus in Born approximation the scattering amplitude is simply the Fourier transform of the potential.

For elastic scattering $k = k'$ holds and thus $\vec{k} \cdot \vec{k}' = k^2 \cos\theta$. Hence we get

$$
\begin{aligned}
\Delta^2 &= |\vec{\Delta}|^2 = 2k^2 - 2\vec{k} \cdot \vec{k}' \\
&= 2k^2 \left(1 - \cos\theta\right) \\
&= 4k^2 \sin^2 \frac{\theta}{2} , \\
\Rightarrow \Delta &= 2k \sin \frac{\theta}{2} .
\end{aligned}
\tag{151}
$$

Therefore the Born scattering amplitude for a central potential reads

$$
\begin{aligned}
f^B(k, \theta, \phi) &= -\frac{1}{4\pi} \int_0^\infty dr\, r^2 U(r) \int_0^\pi d\theta' \sin\theta' \int_0^{2\pi} d\phi\, e^{i\Delta r \cos\theta'} \tag{152} \\
&= -\frac{1}{2} \int_0^\infty dr\, r^2 U(r) \int_{-1}^{+1} d\cos\theta'\, e^{i\Delta r \cos\theta'} \tag{153} \\
&= -\frac{1}{\Delta} \int_0^\infty dr\, r \sin(\Delta r) U(r) . \tag{154}
\end{aligned}
$$

6.3 The Coulomb potential

Taking the **Yukawa potential** as an example

$$U_Y(r) = U_0 \frac{e^{-\alpha r}}{r} , \tag{155}$$

we get

$$f_Y^B = -\frac{U_0}{\alpha^2 + \Delta^2} \tag{156}$$

and thus

$$\frac{d\sigma^B}{d\Omega} = \frac{U_0^2}{(\alpha^2 + \Delta^2)^2} . \tag{157}$$

The **Coulomb potential** can be considered as a special case of the Yukawa potential

$$U_C(r) \;=\; U_0 \frac{1}{r} \tag{158}$$

and we get

$$f_C^B \;=\; -\frac{U_0}{\Delta^2} \;, \tag{159}$$

leading to the famous Rutherford scattering formula

$$\frac{d\sigma^B}{d\Omega} \;=\; \frac{U_0^2}{\Delta^4} \tag{160}$$

$$=\; \left(\frac{q_A q_B}{4\pi\epsilon_0}\right)^2 \frac{1}{16E^2 \sin^4 \frac{\theta}{2}} \;. \tag{161}$$

6.4 Propagator

The Green's function in

$$\Psi_n(\vec{r}) \;=\; e^{i\vec{k}\cdot\vec{r}} + \int G_0(k, \vec{r} - \vec{r}\,')U(\vec{r}\,')e^{i\vec{k}\cdot\vec{r}\,'}d\vec{r}\,'$$

$$+ \int G_0(k, \vec{r} - \vec{r}\,')U(\vec{r}\,') \int G_0(k, \vec{r}\,' - \vec{r}\,'')U(\vec{r}\,'')e^{i\vec{k}\cdot\vec{r}\,''}d\vec{r}\,''d\vec{r}\,'$$

$$+... \tag{162}$$

is also called **propagator**. **Feynman diagrams** are a graphical display of the terms in Eq.(162). The first term corresponds to no interaction, the second term to an interaction at $\vec{r}\,'$ and a propagation from $\vec{r}\,'$ to $\vec{r}$. The third term to an interaction at $\vec{r}\,''$, a propagation from $\vec{r}\,''$ to $\vec{r}\,'$, an interaction at $\vec{r}\,'$ and a propagation from $\vec{r}\,'$ to $\vec{r}$, a.s.o.

- *To repeat this lecture:* Chapter [13.6] of [1]

- *To prepare for next lecture:* Chapter [13.7] of [1]

7 Advanced Topics in Scattering

7.1 Form factor

Assume that the potential is given by an extended distribution of electric charge. Considering the interaction of this distribution with another charge e we have the following potential

$$V(\vec{r}) = \int \frac{Ze^2}{s} \rho(r') d\vec{r'} \,, \tag{163}$$

with $\vec{s} = \vec{r} - \vec{r'}$. For the scattering amplitude we obtain

$$
\begin{aligned}
f(k, \theta) &= -\frac{m}{2\pi\hbar^2} \int e^{i\vec{\Delta}\cdot\vec{r}} \int \frac{Ze^2}{s} \rho(r') d\vec{r'} d\vec{r} \tag{164} \\
&= -\frac{mZe^2}{2\pi\hbar^2} \int e^{i\vec{\Delta}\cdot(\vec{r'}+\vec{s})} \int \frac{1}{s} \rho(r') d\vec{r'} d\vec{r} \tag{165} \\
&= -\frac{mZe^2}{2\pi\hbar^2} \int e^{i\vec{\Delta}\cdot\vec{r'}} \rho(r') d\vec{r'} \int e^{i\vec{\Delta}\cdot\vec{s}} \frac{1}{s} d\vec{r} \tag{166} \\
&= -\frac{mZe^2}{2\pi\hbar^2} \tilde{\rho}(\vec{k} - \vec{k'}) \int e^{i\vec{\Delta}\cdot\vec{s}} \frac{1}{s} d\vec{s} \tag{167} \\
&= \tilde{\rho}(\vec{k} - \vec{k'}) f_{Rutherford}(k, \theta) \,. \tag{168}
\end{aligned}
$$

The Fourier transform of the charge distribution, $\tilde{\rho}$, is called the **form factor** of the extended object. This is a very general result: the cross-section of an extended object is given by the cross-section of the corresponding point like object times the form factor squared.

$$\frac{d\sigma_{Extended}}{d\Omega} = |\tilde{\rho}|^2 \frac{d\sigma_{Point-like}}{d\Omega} \,. \tag{169}$$

The Fourier transformation of the charge distribution can now be obtained by comparing the measurement of the differential cross section with the calculation of the corresponding point-like cross section.

7.2 Electron scattering on nucleon

Thus information about the size of a nucleon or more generally about the charge distribution of a nucleon can be obtained by investigating the scattering of electrons and nucleon. For a realistic investigation, however, more effects have to be taken into account:

a) Scattering of an electron at a static, fixed potential

$$\boxed{\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{Rutherford} .}$$

b) Electron has spin $1/2$

$$\boxed{\left(\frac{d\sigma}{d\Omega}\right)^{*}_{Mott} = \left(\frac{d\sigma}{d\Omega}\right)_{Rutherford} \left(1 - \beta^2 \sin^2 \frac{\theta}{2}\right) ,}$$

with $\beta = v/c$.

c) Finite mass of the nucleon

$$\boxed{\left(\frac{d\sigma}{d\Omega}\right)_{Mott} = \left(\frac{d\sigma}{d\Omega}\right)^{*}_{Mott} \frac{E'}{E} .}$$

Four momentum transfer: $q^2 = (p - p')^2 \approx \frac{4EE'}{c^2} \sin^2 \frac{\theta}{2}$; $Q^2 := -q^2$.

d) The nucleon has a magnetic moment

$$\boxed{\left(\frac{d\sigma}{d\Omega}\right)_{s=1/2-Point} = \left(\frac{d\sigma}{d\Omega}\right)_{Mott} \left[1 + 2\tau \tan^2 \frac{\theta}{2}\right] ,}$$

with $\tau = Q^2/(4M^2c^2)$.

e) The nucleon has an anomalous magnetic moment ($g \neq 2$) and it is extended (form factor).

$$\mu_p = \frac{g_p}{2}\mu_N = +2.79\mu_N = G^p_M(Q^2 = 0) ,$$

$$\mu_n = \frac{g_n}{2}\mu_N = -1.91\mu_N = G^n_M(Q^2 = 0) ,$$

$$\text{nuclear magneton: } \mu_N = \frac{eh}{2m_p} = \frac{m_e}{m_p}\mu_B .$$

One would expect the following structure:

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Mott} F^2(Q^2) \left[1 + 2\tau \tan^2\frac{\theta}{2}\right] ,$$

with $F(0) = g/2$.

The electric charge and the magnetic current have, however, different distributions, thus we get two different form factors. Due to historic reasons one writes:

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Mott} \left[\frac{G_E^2(Q^2) + \tau G_M^2(Q^2)}{1 + \tau} + 2\tau G_M^2(Q^2) \tan^2\frac{\theta}{2}\right] .$$

<div align="right">Rosenbluth-formula (1955)</div>

Experimental investigations have given the following results:

$$G_E^p(Q^2) = \frac{G_M^p(Q^2)}{2.79} = \frac{G_M^n(Q^2)}{-1.91} = G^{Dipole}(Q^2) ,$$

$$G^{Dipole}(Q^2) = \frac{1}{\left(1 + \frac{Q^2}{0.71 \mathrm{GeV}^2}\right)^2} ,$$

$$G_E^n(Q^2) \approx 0 .$$

In the end one gets e.g. information about the structure and the size of a proton: it turns out that a good fit for the charge density of the nucleon is given by a Fermi distribution

$$\rho(r) = \rho_0 \frac{1}{1 + exp\left[\frac{r-R}{a}\right]} , \tag{170}$$

with $R \approx 1fm$, $a \approx 0.5fm$ and $\rho_0 \approx 3 \cdot 10^{17}\mathrm{kg/m^3}$.

A state-of-the quantum field theoretical investigation of nucleon form factors can e.g. be found in [20].

7.3 Collisions between identical particles

<div align="center">— Chapter [13.7] of [1] —</div>

If we consider the scattering of two identical particles, then an event with the angular coordinates (θ, ϕ) cannot be distinguished from an event with

<div align="center">39</div>

the angular coordinates $(\pi - \theta, \pi + \phi)$. Thus interference can occur and the corresponding scattering amplitudes have to be added. We get for the differential cross section (for finding a particle at (θ, ϕ)

$$
\begin{aligned}
\frac{d\sigma}{d\Omega} &= |f(\theta, \phi) + f(\pi - \theta, \pi + \phi)|^2 \quad (171) \\
&= |f(\theta, \phi)|^2 + |f(\pi - \theta, \pi + \phi)|^2 + 2\Re\left(f(\theta, \phi)f^*(\pi - \theta, \pi + \phi)\right) , \quad (172)
\end{aligned}
$$

which differs from the classical expectation of

$$
\frac{d\sigma_{Classic}}{d\Omega} = |f(\theta, \phi)|^2 + |f(\pi - \theta, \pi + \phi)|^2 . \quad (173)
$$

7.3.1 Two spin-less bosons

7.3.2 Two spin 1/2 fermions

- *To repeat this lecture:* Chapter [13.7] of [1]

- *To prepare for next lecture:* Chapter [13.8] of [1]

7.4 Introduction to multichannel scattering

— Chapter [13.8] of [1] —

7.4.1 Elastic Scattering

7.4.2 Inelastic Scattering

- *To repeat this lecture:* Chapter [13.8] of [1]

- *To prepare for next lecture:* Chapter [14.1/2/3] of [1]

8 The density matrix

8.1 Definition

Quantum statistical mechanics is a combination of statistical mechanics and quantum mechanics. In this case we have two sources for the necessity of a statistical description:

- A practical necessity because of a huge number of systems or degrees of freedom. Having an infinite amount of computing power, we simply could overcome this problem and we would not need a statistical description.

- An unavoidable necessity because of the inherent probability character of quantum mechanics. This problem cannot be overcome, even with infinite computer power.

We start our discussion of quantum statistical mechanics with some definitions:

A system that can be described by a single wave function (state vector) is said to be in a **pure state**. One implicitly assumes that a complete set of commuting observables has been determined, which is called a maximal measurement. Basically all systems we were considering till now are in a pure state.

If in a system only non-maximal measurements are or can be made, then the wave function is not completely known and we speak of a **mixed state**. Now a statistical mixture of wave functions must be used to describe the system - this is one of the topics of quantum statistical mechanics.

Another way of stating this difference: for a pure state all sub-systems are in the same state, while for a mixed state the sub-systems can be in different states.

To make these definitions a little more clear, we consider:

- An ensemble of N sub-systems $\alpha = 1, 2, ..., N$.

- Each sub-system is in a pure state described by the state vector $\Psi^{(\alpha)}$ or $|\alpha\rangle$ in Dirac notation.
  The $|\alpha\rangle$ are normalised to one, but they are not necessarily orthogonal.

$$\langle\alpha|\alpha\rangle = 1 . \tag{174}$$

- Choose a complete set of basis vectors $|n\rangle$, i.e. orthogonal eigen vectors of some complete set of operators:

$$\langle n|n'\rangle = \delta_{n,n'} \tag{175}$$

or

$$\langle n|n'\rangle = \delta(n - n') \,, \tag{176}$$

if n is a continuous variable.

Completeness tells us

$$1 = \sum_n |n\rangle\langle n| \,. \tag{177}$$

The pure state $|\alpha\rangle$ can be expanded in terms of the basis $|n\rangle$:

$$|\alpha\rangle = \sum_n c_n^{(\alpha)}|n\rangle \,, \tag{178}$$

with

$$c_n^{(\alpha)} = \langle n|\alpha\rangle \,, \tag{179}$$

$$\sum_n \left|c_n^{(\alpha)}\right|^2 = 1 \,. \tag{180}$$

Next we consider an observable represented by an operator A. The expectation value of A in the state $|\alpha\rangle$ is

$$\langle A\rangle_\alpha = \langle \alpha|A|\alpha\rangle \tag{181}$$

$$= \sum_n \sum_{n'} c_{n'}^{(\alpha)*} c_n^{(\alpha)} \langle n'|A|n\rangle \tag{182}$$

$$= \sum_n \sum_{n'} \langle n|\alpha\rangle\langle \alpha|n'\rangle\langle n'|A|n\rangle \,. \tag{183}$$

The average of A over the ensemble - the **ensemble** or **statistical average** is denoted by

$$\langle A\rangle = \sum_{\alpha=1}^N W_\alpha \langle A\rangle_\alpha \,, \tag{184}$$

with W_α being the **statistical weight** of the pure state $|\alpha\rangle$, i.e. the probability of finding the whole system in the state $|\alpha\rangle$:

$$0 \le W_\alpha \le 1 \,, \tag{185}$$

$$\sum_{\alpha=1}^N W_\alpha = 1 \,. \tag{186}$$

All in all we can now write

$$
\langle A \rangle \;=\; \sum_{\alpha=1}^{N} \sum_{n} \sum_{n'} \langle n|\alpha\rangle W_\alpha \langle \alpha|n'\rangle \langle n'|A|n\rangle \tag{187}
$$

$$
=\; \sum_{n} \sum_{n'} \langle n|\rho|n'\rangle \langle n'|A|n\rangle \tag{188}
$$

$$
=\; \sum_{n} \langle n|\rho A|n\rangle \tag{189}
$$

$$
=\; \mathrm{Tr}(\rho \mathrm{A}) \;, \tag{190}
$$

with the **density operator** or **statistical operator**, being defined as

$$
\rho = \sum_{\alpha=1}^{N} |\alpha\rangle W_\alpha \langle \alpha| \;. \tag{191}
$$

Remarks:

- The knowledge of the density operator enables us to calculate ensemble averages.

- Taking A to be the unit operator and keeping in mind that the pure states are normalised to one, we have

$$
\mathrm{Tr}(\rho) = 1 \;. \tag{192}
$$

If the states $|\alpha\rangle$ are not normalised to one, we get

$$
\langle A \rangle = \frac{\mathrm{Tr}(\mathrm{A}\rho)}{\mathrm{Tr}(\rho)} \;. \tag{193}
$$

- The density operator can also be expressed in terms of matrix elements - the **density matrix**.

    - Definition:

$$
\rho_{nn'} \;=\; \langle n|\rho|n'\rangle \tag{194}
$$

$$
=\; \sum_{\alpha=1}^{N} \langle n|\alpha\rangle W_\alpha \langle \alpha|n'\rangle \tag{195}
$$

$$
=\; \sum_{\alpha=1}^{N} W_\alpha c_{n'}^{(\alpha)*} c_{n}^{(\alpha)} \;. \tag{196}
$$

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– Diagonal elements: the diagonal elements of the density matrix

$$\rho_{nn} = \langle n|n \rangle = \sum_{\alpha=1}^{N} W_\alpha \left| c_n^{(\alpha)} \right|^2 \qquad (197)$$

have the following interpretation:

W_α is the probability of finding the whole system in the state $|\alpha\rangle$ and $\left| c_n^{(\alpha)} \right|^2$ is the probability of finding that $|\alpha\rangle$ to be in the state $|n\rangle$. Thus ρ_{nn} gives the probability of finding the ensemble in the state $|n\rangle$.

Moreover we have

$$0 \le \rho_{nn} \le 1 . \qquad (198)$$

The l.h.s. follows from Eq.(197) and the r.h.s. from Eq.(192).

– Hermiticity: the density matrix is hermitian

$$\langle n|\rho|n' \rangle = \langle n'|\rho|n \rangle^* . \qquad (199)$$

Thus it can be diagonalised by a unitary transformation. If we choose a representation $|k\rangle$ where ρ is diagonal, then we have

$$\rho_{kk'} = \rho_{kk}\delta_{kk'} . \qquad (200)$$

In that basis we immediately see from Eq.(198)

$$\text{Tr}(\rho^2) \le \text{Tr}(\rho) = 1 . \qquad (201)$$

This relation is also valid in any other representation, since the trace is invariant under unitary transformations. Thus we have

$$\sum_n \sum_{n'} |\rho_{nn'}|^2 \le 1 . \qquad (202)$$

Now let us assume that the whole system is in a pure state $|\lambda\rangle$, meaning $W_\alpha = \delta_{\alpha\lambda}$. So the density operator reads

$$\rho^\lambda = |\lambda\rangle\langle\lambda| , \qquad (203)$$

which is simply a projection operator with

$$(\rho^\lambda)^2 = \rho^\lambda . \qquad (204)$$

Hence Eq.(201) becomes for a pure state

$$\text{Tr}(\rho^\lambda)^2 = \text{Tr}(\rho\lambda) = 1 . \qquad (205)$$

This is now a new criterion for deciding whether a state was pure or not!

$$\mathrm{Tr}(\rho)^2 = 1 \quad \Rightarrow \text{state is pure} , \tag{206}$$
$$\mathrm{Tr}(\rho)^2 < 1 \quad \Rightarrow \text{state is mixed} . \tag{207}$$

If the system is in a pure state we have also

$$\langle A \rangle = \langle \lambda | A | \lambda \rangle . \tag{208}$$

If we use a diagonal representation in that case we get in addition

$$\rho^{\lambda}_{kk'} = \delta_{k\lambda}\delta_{k'\lambda} . \tag{209}$$

Thus one diagonal element is one and the rest zero.

- The indices n, n' denote all possible quantum numbers, if we are e.g. only interested in spin, we have a **reduced density matrix**.

8.2 Polarisation

8.3 Von-Neumann equation

In the Schrödinger-picture we have at the time t_0

$$\rho(t_0) = \sum_{\alpha=1}^{N} W_\alpha |\alpha(t_0)\rangle\langle\alpha(t_0)| . \tag{210}$$

The time evolution of the states is given as

$$|\alpha(t)\rangle = U(t,t_0)|\alpha(t_0)\rangle , \tag{211}$$

with

$$U(t,t_0) = e^{-i\frac{H}{\hbar}(t-t_0)} \tag{212}$$

for a time-independent Hamiltonian. Thus the density operator at time t is given as

$$\rho(t) = \sum_{\alpha=1}^{N} W_\alpha |\alpha(t)\rangle\langle\alpha(t)| \tag{213}$$
$$= U(t,t_0)\rho(t_0)U^\dagger(t,t_0) \tag{214}$$
$$= e^{-i\frac{H}{\hbar}(t-t_0)}\rho(t_0)e^{+i\frac{H}{\hbar}(t-t_0)} . \tag{215}$$

This last equation is equivalent to

$$i\hbar \frac{\partial}{\partial t}\rho(t) = [H, \rho(t)] \ , \tag{216}$$

which is called the **von-Neumann-equation** or sometimes also .**Liouville-von-Neumann-equation**

Remarks:

- Eq.(216) is the equivalent of the **Liouville-equation** for the phase space probability in classical mechanics.

$$\frac{d}{dt}\rho = \{H, \rho\} \ . \tag{217}$$

- Eq.(216) looks also similar to the **Heisenberg equation** of motion for an observable,

$$i\hbar \frac{d}{dt} A_H = -[H, A_H] + i\hbar \frac{\partial}{\partial t} A_H \ , \tag{218}$$

but keep in mind that in Eq.(216) the states are given in the Schrödinger-picture.

- The time evolution of the statistical average of an operator A that is not explicitly time-dependent reads

$$\begin{align}
\frac{\partial}{\partial t}\langle A\rangle &= \frac{\partial}{\partial t}\mathrm{Tr}\,(\rho A) \tag{219}\\
&= \mathrm{Tr}\left(A\frac{\partial}{\partial t}\rho\right) \tag{220}\\
&= -\frac{i}{\hbar}\mathrm{Tr}\,(A\,[H,\rho]) \tag{221}\\
&= -\frac{i}{\hbar}\mathrm{Tr}\,(AH\rho - A\rho H) \tag{222}\\
&= -\frac{i}{\hbar}\mathrm{Tr}\,([A,H]\,\rho) \ . \tag{223}
\end{align}$$

- The density operator in the Schrödinger-picture is time-dependent!

- *To repeat this lecture:* Chapter [14.1/2/3] of [1]

- *To prepare for next lecture:* Chapter [14.4/5] of [1]

9 Quantum mechanical ensembles

<center>— Chapter [14.4/5] of [1] —</center>

In the following we will discuss different classes of ensembles. We consider only systems in thermal equilibrium, thus the averages of physical observables are constant. In that case we get a time-independent density matrix

$$\frac{\partial}{\partial t}\rho = 0 \; , \tag{224}$$

which is equivalent to H having no explicit time dependence and

$$[H, \rho] = 0 \; . \tag{225}$$

Now we can choose a basis $|n\rangle$ in which both H and ρ are diagonal

$$\langle n|H|m\rangle \;\; = \;\; H_{nm} = E_n \delta_{nm} \; , \tag{226}$$
$$\langle n|\rho|m\rangle \;\; = \;\; \rho_{nm} = \rho_{nn} \delta_{nm} \; . \tag{227}$$

The probability that a sub-system chosen randomly from the ensemble is in the eigenstate $|n\rangle$ is ρ_{nn}. Since ρ can be expressed in terms of H

$$\rho = \rho(H) \; , \tag{228}$$

we can also express ρ_{nn} in terms of E_N.

Below we present different functional dependencies of ρ_{nn} from E_n, which define different ensembles.

9.1 Micro-canonical ensemble

A micro-canonical ensemble describes a closed system, i.e. we have for each sub-system:

- a fixed number of particles $\mathcal{N}$;

- a fixed volume $\mathcal{V}$;

- the energy E lies in the small interval

$$E_0 \leq E \leq E_0 + \Delta \; .$$

<u>Notation:</u>

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- Γ: the total number of distinct pure states in which a member of the ensemble can be found

$$\Gamma = \Gamma(\mathcal{N}, \mathcal{V}, E_0, \Delta) \ .$$

- $\mathcal{H}$: the Hamiltonian of each sub-system.

Now we make the **fundamental postulates:**

1. There is an equal probability of finding the system in any of these states, i.e.

$$\rho_{nn} = \begin{cases} 1/\Gamma & \text{for } E_0 \leq E \leq E_0 + \Delta \\ 0 & \text{else} \end{cases} \ . \qquad (229)$$

2. The members of the ensemble do not interact, so the corresponding wave functions do not interfere. This can be obtained by demanding, that the wave functions of each member $|\alpha\rangle$ of the ensemble are distributed at random or equally: the phases of the probability amplitudes $c_n^{(\alpha)}$ are distributed at random.

The **entropy** of the system, is defined as

$$S = k_B \log \Gamma \ , \qquad (230)$$

with the Boltzmann constant $k_B = 1.3806488(13) \cdot 10^{-23} \text{J K}^{-1}$.

<u>Remarks:</u>

- The definition agrees with the usual thermodynamical one, but now Γ is calculated within using quantum mechanics.

- If each sub-system is in the same state we have $\Gamma = 1$ and thus $S = 0$ and the system is perfectly ordered.

- If Γ is greater than 1, the system is disordered. Thus S is a measure of disorder.

The entropy has the familiar properties:

1. The entropy of a closed system is maximal, when the system is in equilibrium.

2. The entropy is additive, i.e. if a closed system is divided into parts with the entropy S_1 and S_2 we have $S = S_1 + S_2$.

3. The temperature T of the system is defined as

$$\frac{1}{T} = \frac{\partial S}{\partial E} \ . \tag{231}$$

In practice the micro-canonical ensemble is difficult to use, thus Gibbs introduced two additional concepts: the canonical ensemble and the grand canonical ensemble.

9.2 Canonical ensemble

Definition:

- In this case the investigated system $\mathcal{S}$ is in thermal contact with a much larger heat reservoir $\mathcal{R}$. The combined system $\mathcal{S} + \mathcal{R}$ is closed and its statistical properties are defined by the micro-canonical ensemble.

- The system $\mathcal{S}$ is composed of a fixed number of particles $\mathcal{N}_\mathcal{S}$ within a volume $\mathcal{V}_\mathcal{S}$ and it is in the energy eigenstate $E_\mathcal{S}$. The system $\mathcal{R}$ is composed of a fixed number of particles $\mathcal{N}_\mathcal{R}$ within a volume $\mathcal{V}_\mathcal{R}$ and it is in the energy eigenstate $E_\mathcal{R}$.

- The systems $\mathcal{S}$ and $\mathcal{R}$ are in contact and can thus exchange energy - the interaction is supposed to be so weak, that at any time $\mathcal{S}$ and $\mathcal{R}$ are in definite energy eigenstates with energies $E_\mathcal{R}$ and $E_\mathcal{S}$.

- In equilibrium $\mathcal{S}$ and $\mathcal{R}$ have a common temperature T.

- Conservation of energy tells us

$$E = E_\mathcal{R} + E_\mathcal{S} \ , \tag{232}$$

where E is an eigenvalue of the combined system. Since the whole system is described by the micro-canonical ensemble we have

$$E_0 \leq E \leq E_0 + \Delta \ \text{ with } \ \Delta \ll E_0 \ .$$

Problem: Determine the probability that at a given temperature T the system $\mathcal{S}$ is to be found in a state with energy $E_\mathcal{S}$.

Solution:

- $d\Gamma(E)$: total number of distinct states of the combined system with energies in $[E, E + dE]$.

- The probability of finding the combined system with energies in $[E, E + dE]$ is
$$dP = \begin{cases} C d\Gamma(E) & E_0 \leq E \leq E_0 + \Delta \\ 0 & \text{else} \end{cases}, \qquad (233)$$
where C is a constant describing the probability of finding one state.

- Denoting the corresponding numbers in the system $\mathcal{S}$ and $\mathcal{R}$ by $d\Gamma_\mathcal{S}$ and $d\Gamma_\mathcal{R}$, we have
$$d\Gamma = d\Gamma_\mathcal{S} d\Gamma_\mathcal{R}, \qquad (234)$$
$$dP = C d\Gamma_\mathcal{S}(E_\mathcal{S}) d\Gamma_\mathcal{R}(E_\mathcal{R}) \delta(E - E_\mathcal{S} - E_\mathcal{R}), \qquad (235)$$
where the δ-function expresses the energy conservation.

- dP_n is the probability that the system $\mathcal{S}$ has the energy E_n without regard to the state of the reservoir (i.e. we are summing over all the states in the reservoir that yield the same E_n)
$$dP_n = C d\Gamma_\mathcal{S}(E_n) \int \delta(E - E_n - E_\mathcal{R}) d\Gamma_\mathcal{R}(E_\mathcal{R}) \qquad (236)$$
$$= C d\Gamma_\mathcal{S}(E_n) \Delta\Gamma_\mathcal{R}(E - E_n), \qquad (237)$$
with $\Delta\Gamma_\mathcal{R}(E - E_n)$ being the total number of states in the reservoir, subject to the conservation of energy.

- The corresponding entropy of the reservoir is given as
$$S_\mathcal{R} = k_B \log \Delta\Gamma_\mathcal{R}, \qquad (238)$$
$$\Delta\Gamma_\mathcal{R} = e^{\frac{S_\mathcal{R}}{k_B}}. \qquad (239)$$

- Since the system $\mathcal{S}$ is supposed to be very small compared to the total system, we have $E_n \ll E$ and thus we can Taylor expand:
$$S_\mathcal{R}(E_\mathcal{R}) = S_\mathcal{R}(E - E_n) \qquad (240)$$
$$= S_\mathcal{R}(E) - \frac{\partial S_\mathcal{R}(E)}{\partial E} E_n + \dots \qquad (241)$$
$$= S_\mathcal{R}(E) - \frac{E_n}{T} + \dots. \qquad (242)$$

- Putting now the pieces together we get
$$dP_n = C d\Gamma_\mathcal{S}(E_n) \Delta\Gamma_\mathcal{R}(E - E_n) \qquad (243)$$
$$= C d\Gamma_\mathcal{S}(E_n) e^{\frac{S_\mathcal{R}(E - E_n)}{k_B}} \qquad (244)$$
$$= C d\Gamma_\mathcal{S}(E_n) e^{\frac{S_\mathcal{R}(E)}{k_B}} e^{-\frac{E_n}{k_B T}} \qquad (245)$$
$$= \mathcal{A} e^{-\frac{E_n}{k_B T}} d\Gamma_\mathcal{S}(E_n). \qquad (246)$$

This is already the desired result: the probability of finding the system $\mathcal{S}$ in the energy state with E_n is given by $\mathcal{A}e^{-\frac{E_n}{k_B T}}$.

- Thus we can write the density matrix as

$$\rho_{nm} = \mathcal{A}e^{-\beta E_n}\delta_{nm} \ , \tag{247}$$

with $\beta = 1/(k_B T)$.

Remarks:

1. The coefficient $\mathcal{A}$ can be extracted from the condition $\mathrm{Tr}(\rho) = 1$.

$$
\begin{align}
1 &= \sum_n \rho_{nn} \tag{248} \\
&= \sum_n \mathcal{A}e^{-\beta E_n} \tag{249} \\
\Rightarrow \mathcal{Q}_{\mathcal{N}_S} := \mathcal{A}^{-1} &= \sum_n e^{-\beta E_n} = \mathrm{Tr}\left[e^{-\beta H}\right] . \tag{250}
\end{align}
$$

$\mathcal{Q}_{\mathcal{N}_S}$ is called the **partition function**.

2. The sum runs over all distinct states, which is not necessarily the same as over all energy eigenstates.

3. The density operator can now be written as

$$\rho = \frac{e^{-\beta H}}{\mathcal{Q}_{\mathcal{N}_S}} \ . \tag{251}$$

4. The ensemble average of an operator A is now given as

$$
\begin{align}
\langle A \rangle &= \mathrm{Tr}(\rho A) \tag{252} \\
&= \frac{1}{\mathcal{Q}_{\mathcal{N}_S}}\mathrm{Tr}\left(e^{-\beta H}A\right) \tag{253} \\
&= \frac{\mathrm{Tr}\left(e^{-\beta H}A\right)}{\mathrm{Tr}\left[e^{-\beta H}\right]} \ . \tag{254}
\end{align}
$$

5. The average energy $\bar{E}$ of the system can be found by setting $A = H$. Using Eq.(250) it can also be expressed as

$$\bar{E} = \langle H \rangle = -\frac{1}{\mathcal{Q}_{\mathcal{N}_S}}\frac{\partial \mathcal{Q}_{\mathcal{N}_S}}{\partial \beta} = -\frac{\partial}{\partial \beta}\log \mathcal{Q}_{\mathcal{N}_S} \ . \tag{255}$$

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9.3 Grand canonical Ensemble

This is similar the canonical ensemble, but now we allow in addition the exchange of particles between the system $\mathcal{S}$ and the reservoir $\mathcal{R}$. The total number of particles

$$\mathcal{N} = \mathcal{N}_\mathcal{R} + \mathcal{N}_\mathcal{S} \tag{256}$$

is constant.

All derivations are similar up to difference in the Taylor expansion of the entropy, where now the change of particle numbers is taken into account.

$$
\begin{aligned}
\mathcal{S}_\mathcal{R}(E - E_n, \mathcal{N} - \mathcal{N}_\mathcal{S}) &= \mathcal{S}_\mathcal{R}(E, \mathcal{N}) \\
&\quad - \frac{\partial \mathcal{S}_\mathcal{R}(E, \mathcal{N})}{\partial E} E_n(\mathcal{N}_\mathcal{S}) - \frac{\partial \mathcal{S}_\mathcal{R}(E, \mathcal{N})}{\partial \mathcal{N}} \mathcal{N}_\mathcal{S} + \dots \; . \\
&= \mathcal{S}_\mathcal{R}(E, \mathcal{N}) - \frac{E_n(\mathcal{N}_\mathcal{S})}{T} + \frac{\mu}{T} \mathcal{N}_\mathcal{S} + \dots \; .
\end{aligned}
\tag{257}
$$

The density matrix gets now the form

$$\rho_{nm} = \mathcal{B} e^{[-\beta E_n(\mathcal{N}_\mathcal{S}) - \alpha \mathcal{N}_\mathcal{S}]} \delta_{nm} \; , \tag{258}$$

with $\mathcal{B}$ being a constant and $\alpha = (\partial \mathcal{S}_\mathcal{R}/\partial \mathcal{N}/k_B)$. $\mu = -\alpha/\beta$ is called **chemical potential**.

In order to give an operator form of the density operator, we introduce the number operator $\nu_\mathcal{S}$, that is counting the number of particles in the system $\mathcal{S}$. Its eigenvalues are $N = 0, 1, 2, \dots$. Thus we get for the density operator

$$\rho = \mathcal{B} e^{-\beta H(\nu_\mathcal{S}) - \alpha \nu_\mathcal{S}} \; . \tag{259}$$

The constant $\mathcal{B}$ can again be determined from $\mathrm{Tr}(\rho) = 1$ and we get

$$\mathcal{B}^{-1} := Z(\alpha, T) = \mathrm{Tr}\left[e^{-\beta H(\nu_\mathcal{S}) - \alpha \nu_\mathcal{S}} \right] \; . \tag{260}$$

Z is called the **grand partition function** and we can write

$$
\begin{aligned}
Z(\alpha, T) &= \sum_N \sum_n e^{-\beta E_n(N) - \alpha N} \tag{261} \\
&= \sum_N \left[\sum_n e^{-\beta E_n(N)} \right] e^{-\alpha N} \tag{262} \\
&= \sum_N \left[\sum_n e^{-\beta E_n(N)} \right] \left[e^{-\alpha} \right]^N \tag{263} \\
&= \sum_N \mathcal{Q}_N(T) z^N \; , \tag{264}
\end{aligned}
$$

where $z = exp(-\alpha)$ is called **fugacity** and $\mathcal{Q}_N(T)$ is the partition function of a system of N particles.

9.4 Spin 1/2 particle in a magnetic field

9.5 Average of a particle in a box

- *To repeat this lecture:* Chapter [14.4/5] of [1]

- *To prepare for next lecture:* Chapter [14.6] of [1]

10   Systems of non-interacting particles

We discuss now systems of large numbers of non-interacting objects (particles) which are equivalent and possess the same energy levels.
$E_j(j = 1, 2, 3, ..)$ denotes an energy level of one of the particles. The total energy E of the system can be written as

$$E_{\mathcal{S}} = E = \sum_j n_j E_j \ , \tag{265}$$

where the sum runs over all energy eigenstates and n_j is the number of particles having the same energy E_j. The total number of particles in the system is

$$N_{\mathcal{S}} = N = \sum_j n_j \ . \tag{266}$$

The individual particle numbers can have the following values:

$$n_j = \begin{cases} 0, 1, 2, 3, ... & \text{Maxwell-Boltzmann} & \text{particles distinguishable} \\ 0, 1, 2, 3, ... & \text{Bose-Einstein} & \text{particles indistinguishable - bosons} \\ 0, 1 & \text{Fermi-Dirac} & \text{particles indistinguishable - fermions} \end{cases} \ . \tag{267}$$

For obtaining the partition functions we have to sum over all distinct states and not only over all energy eigenstates. Thus we need to know the number of distinct states g_E having the same energy E.
To find that we start by looking at the total wave function of a system and we find

$$\Psi = \begin{cases} \Phi_{E_j}(1)\Phi_{E_k}(2) \cdot \cdots \cdot \Phi_{E_l}(N) & \text{Maxwell-Boltzmann} \\ \text{total symmetric} & \text{Bose-Einstein} \\ \text{total antisymmetric} & \text{Fermi-Dirac} \end{cases} \ . \tag{268}$$

This leads to

$$g_E = \begin{cases} g_E^{MB} = \frac{N!}{\Pi_j(n_j!)} & \text{Maxwell-Boltzmann} \\ g_E^{BE} = 1 & \text{Bose-Einstein} \\ g_E^{FD} = 0, 1 & \text{Fermi-Dirac} \end{cases} \ . \tag{269}$$

Remarks:

- ad MB: If all energies $E_j, E_k, ..., E_l$ are different, then each energy level is $N!$-fold degenerate. If, however, n_j particles with $n_j > 1$ have the same energy, then an interchange among them does not change the wave function.

- ad BE: there is only one total symmetric wave function.

- ad FD: there is only one total anti-symmetric wave function. If $n_j > 1$ then g_E becomes zero.

Now the partition function reads for all the three cases:

$$Q_N(T) = \sum_{\{n_j\}} g_E \exp\left[-\beta \sum_j n_j E_j\right] , \qquad (270)$$

where $\sum_{\{n_j\}}$ denotes a sum over every possible set of numbers n_j that is compatible with the total number N.
The average value of the energy $\langle E \rangle$ of the system can be calculated if the average value $\langle n_i \rangle$ of each occupation number n_i is known.

$$\langle E \rangle = \sum_i E_i \langle n_i \rangle . \qquad (271)$$

$\langle n_i \rangle$ can be determined from the canonical ensemble

$$\langle n_i \rangle = \frac{1}{Q_N(T)} \sum_{\{n_j\}} g_E \exp\left[-\beta \sum_j n_j E_j\right] n_i , \qquad (272)$$

which is equivalent to

$$\langle n_i \rangle = -\frac{\partial \log Q_N(T)}{\partial(\beta E_i)} . \qquad (273)$$

For the case of MB the sum can be performed explicitly to obtain

$$Q_N(T) = \left[\sum_j \exp\left(-\beta E_j\right)\right]^N , \qquad (274)$$

leading to

$$\langle n_i \rangle = \exp\left[-\left(\beta E_i + \alpha\right)\right] , \qquad (275)$$

with

$$\alpha = \log\left[\frac{\sum_j \exp\left(-\beta E_j\right)}{N}\right] . \qquad (276)$$

For the case of BE and FD it is easier to start with the grand partition function

$$Z \; = \; \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \ldots g_E \exp\left\{-\beta \sum_j \left[n_j E_j(N)\right] - \alpha \sum_j n_j\right\} \quad (277)$$

$$= \; \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \ldots g_E \prod_j \exp\left\{-n_j \left[\beta E_j(N) + \alpha\right]\right\} \quad (278)$$

$$= \; \prod_j \sum_{n_j=0}^{\infty} g_E \exp\left\{-n_j \left[\beta E_j(N) + \alpha\right]\right\} . \quad (279)$$

In the case of BE we have $g_E = 1$ and n_j has values from 0 to ∞. Thus we have a simple geometric series and get

$$Z^{BE} \; = \; \prod_j \frac{1}{1 - \exp\left\{-\left[\beta E_j(N) + \alpha\right]\right\}} . \quad (280)$$

In the case of FD we have $g_E = 0, 1$ and n_j has only the values 0 and 1. So we simply can write down the two terms and get

$$Z^{FD} \; = \; \prod_j \left[1 + \exp\left\{-\left[\beta E_j(N) + \alpha\right]\right\}\right] . \quad (281)$$

The average number of states is now given as

$$\langle n_i \rangle \; = \; \frac{1}{Z} \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \ldots g_E \exp\left\{-\beta \sum_j \left[n_j E_j(N)\right] - \alpha \sum_j n_j\right\} n_i \quad (282)$$

$$= \; -\frac{\partial \log Z}{\partial \left[\beta E_i(N)\right]} . \quad (283)$$

Now all three cases (MB, BE and FD) can be expressed with one formula:

$$\langle n_i \rangle \; = \; \frac{1}{\exp\left[\beta E_i(N) + \alpha\right] + \gamma} \quad (284)$$

with

$$\gamma = \begin{cases} 0 & \text{MB} \\ -1 & \text{BE} \\ +1 & \text{FD} \end{cases} . \quad (285)$$

The function

$$\langle n(E) \rangle = \frac{1}{\exp\left[\beta E + \alpha\right] + \gamma} \quad (286)$$

is called the **distribution function**. Plotted as a function of $\beta E + \alpha$ one gets

56
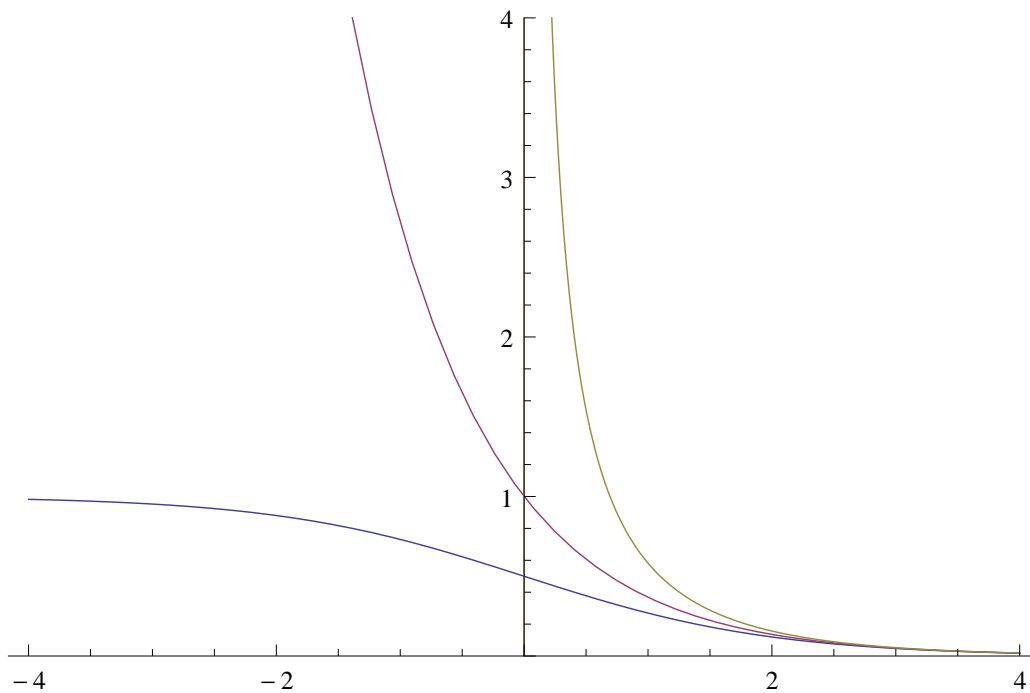
Remarks:

- For large values of $\beta E + \alpha$ all three cases become indistinguishable.

- The FD-distribution cannot exceed one.

- The BE-distribution diverges for $\beta E + \alpha \to 0$. This is the case where Bose-Einstein condensation occurs.

Finally α can be determined from

$$\langle N \rangle = \sum_j \langle n_j \rangle = \sum_j \frac{1}{\exp\left[\beta E_j(N) + \alpha\right] + \gamma} \ . \tag{287}$$

- *To repeat this lecture:* Chapter [14.6] of [1]

- *To prepare for next lecture:* Chapter [15.1] of [1]

11 The Klein-Gordon equation

— Chapter [15.1] of [1] —

11.1 Derivation

Using the **correspondence principle**

$$E \;\to\; i\hbar \frac{\partial}{\partial t} \;, \tag{288}$$

$$\vec{p} \;\to\; \frac{\hbar}{i} \vec{\nabla} \;, \tag{289}$$

the Schrödinger equation can be derived from the non-relativistic energy momentum relation:

$$E \;=\; \frac{\vec{p}^2}{2m} \;, \tag{290}$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \Psi(t,\vec{x}) \;=\; -\frac{\hbar^2 \vec{\nabla}^2}{2m} \Psi(t,\vec{x}) \;. \tag{291}$$

It is a priori clear, that the Schrödinger equation cannot be applied to relativistic energies.

If we want to discuss highly energetic phenomena, like particle accelerators, early universe, black holes,.. we have to start from the relativistic energy momentum relation. This will immediately lead to the **Klein-Gordon equation**, which was derived by Schrödinger (1925), Gordon (1926) and Klein (1927).

$$E^2 \;=\; \vec{p}^2 c^2 + m^2 c^4 \tag{292}$$

$$\Rightarrow -\hbar^2 \frac{\partial^2}{\partial t^2} \Phi(t,\vec{x}) \;=\; (-\hbar^2 c^2 \vec{\nabla}^2 + m^2 c^4) \Phi(t,\vec{x}) \;. \tag{293}$$

The last equation can be rewritten as

$$\boxed{\left[\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \left(\frac{mc}{\hbar} \right)^2 \right] \Phi = 0} \;. \tag{294}$$

<u>Remarks:</u>

- The differential operator appears also e.g. in the wave equation in electro dynamics. It is called **D'Alembert operator** and it is Lorentz invariant. This can be seen by writing

$$\Box = \partial_\mu \partial^\mu = \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x_\mu} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 \;, \tag{295}$$

with $x^\mu = (ct, \vec{x})$, $x_\mu = (ct, -\vec{x})$, $\partial_\mu = \partial/\partial x^\mu = (1/c\ \partial/\partial t, \vec{\nabla})$ and $\partial^\mu = \partial/\partial x_\mu = (1/c\ \partial/\partial t, -\vec{\nabla})$.

Thus (m can be written as $p_\mu p^\mu$ and Φ is assumed to be a scalar) the whole Klein-Gordon equation is Lorentz invariant.

- The Klein-Gordon-equation describes scalar particles like the Higgs-boson.

- The Klein-Gordon-equation, Eq.(294), is a second order equation with respect to time, while the Schrödinger-equation was a first-order equation.

- $\hbar/(mc)$ is the Compton wave length.

11.2 Charged particle in an electromagnetic field

In order to describe a scalar particle with charge q in an electro-magnetic field described by a vector potential $\vec{A}(\vec{r}, t)$ and a scalar potential $\phi(\vec{r}, t)$ we use the **principle of minimal coupling**. This means we make the following replacements[3]

$$E \rightarrow E - q\phi \,, \tag{296}$$

$$\vec{p} \rightarrow \vec{p} - \frac{q}{c}\vec{A} \,. \tag{297}$$

Hence the energy-momentum relating changes to

$$(E - q\phi)^2 = (\vec{p} - \frac{q}{c}\vec{A})^2 c^2 + m^2 c^4 \,, \tag{298}$$

leading to

$$\left(i\hbar\frac{\partial}{\partial t} - q\phi\right)^2 \Phi(t, \vec{x}) = \left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A}\right)^2 c^2 + m^2 c^4\right] \Phi(t, \vec{x}) \,. \tag{299}$$

By making the ansatz

$$\Phi(t, \vec{x}) = \tilde{\Phi}(t, \vec{x}) e^{i\frac{mc^2}{\hbar}t} \tag{300}$$

we split of the rest energy of the particle. If the particle is moving non-relativistic then this is the dominant part of the energy and one can investigate the non-relativistic limit. We will do this in the next section in a slightly modified way.

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[3]In 4-vector notation it reads: $p^\mu \rightarrow p^\mu - \frac{q}{c}A^\mu$, with $A^\mu = (\phi, \vec{A})$.

11.3   Stationary solutions

Now we look for stationary solutions

$$\Phi(\vec{x}, t) =: \Phi(\vec{x})e^{-i\frac{E}{\hbar}t} \,, \tag{301}$$

of the Klein-Gordon equation, given in Eq.(299).
Assuming that $\vec{A}$ and ϕ are time independent, we get

$$(E - q\phi)^2 \, \Phi(\vec{x}) \;=\; \left[\left(\frac{\hbar}{i}\vec{\nabla} - \frac{q}{c}\vec{A} \right)^2 c^2 + m^2 c^4 \right] \Phi(\vec{x}) \,. \tag{302}$$

If we choose in addition $\vec{A} = 0$ and ϕ to be spherical symmetric, we get

$$\left[(E - q\phi)^2 - m^2 c^4 \right] \Phi(\vec{x}) \;=\; -\hbar^2 c^2 \vec{\nabla}^2 \Phi(\vec{x}) \,. \tag{303}$$

Now we can separate the solution in spherical coordinates

$$\Phi(\vec{x}) = R_{El}(r) Y_{lm}(\theta, \phi) \,, \tag{304}$$

leading to

$$-\hbar^2 c^2 \left[\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \right) - \frac{l(l+1)}{r^2} \right] R_{El}(r) \;=\; \left[(E - q\phi(r))^2 - m^2 c^4 \right] R_{El}(r)$$

$$\left[\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \right) - \frac{l(l+1)}{r^2} + \left\{ \left(\frac{E - q\phi(r)}{\hbar c} \right)^2 - \left(\frac{mc}{\hbar} \right)^2 \right\} \right] R_{El}(r) \;=\; 0 \,. \tag{305}$$

Remarks:

- This is the same structure as in the case of the Schrödinger-equation, given in Eq.(54). We get the old result, if we replace the curly bracket by $k^2 - U(r)$.

- For the non-relativistic limit we write the total energy as

$$E = E' + mc^2 \tag{306}$$

and we assume $E' \ll mc^2$ and also $|q\phi| \ll mc^2$. We then have

$$(E - q\phi)^2 - m^2 c^4 \;=\; \left(E' + mc^2 - q\phi \right)^2 - m^2 c^4 \tag{307}$$

$$=\; m^2 c^4 \left[\left(1 + \frac{E' - q\phi}{mc^2} \right)^2 - 1 \right] \tag{308}$$

$$\approx\; 2mc^2 (E' - q\phi) \,. \tag{309}$$

This gives

$$\left[\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) - \frac{l(l+1)}{r^2} + 2\frac{m}{\hbar^2}\left(E' - q\phi(r)\right)\right]R_{El}(r) = 0 , \tag{310}$$

which gives Eq.(54), when we equate

$$k^2 = \frac{2mE'}{\hbar^2} , \tag{311}$$

$$U(r) = \frac{2m}{\hbar^2}q\phi(r) . \tag{312}$$

So we have proven that the non-relativistic limit of the Klein-Gordon equation gives the Schrödinger equation.

11.4 Interpretation

Looking at the Klein-Gordon equation a little more in detail one immediately finds some seemingly inconsistencies.

1. In the same way as it was done for the Schrödinger-equation one can also derive a continuity equation for the case of the Klein-Gordon equation.
$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0 . \tag{313}$$

In this case the probability density $\rho(\vec{r}, t)$ and the probability current density $\vec{j}(\vec{r}, t)$ reads

$$\rho(\vec{r}, t) = \frac{i\hbar}{2mc^2}\left(\Phi^*\frac{\partial \Phi}{\partial t} - \Phi\frac{\partial \Phi^*}{\partial t}\right) , \tag{314}$$

$$\vec{j}(\vec{r}, t) = \frac{\hbar}{2mi}\left(\Phi^*(\vec{\nabla}\Phi) - \Phi(\vec{\nabla}\Phi^*)\right) . \tag{315}$$

Here one easily sees that the probability density can also have negative values, prohibiting a simple interpretation of this quantity.

2. The free Klein-Gordon equation in Eq.(294) can be solved by plane waves
$$\Phi(\vec{r}, t) = Ae^{i(\vec{k}\cdot\vec{r} - \omega t)} . \tag{316}$$

Inserting this ansatz into Eq.(294) one gets

$$\hbar^2\omega^2 = m^2c^4 + \hbar^2c^2k^2 \tag{317}$$

$$\Rightarrow E = \pm\sqrt{m^2c^4 + \hbar^2c^2k^2} . \tag{318}$$

Now we have in principle a positive and a negative energy value; a result that has to be understood somehow.

The source of all these problems lies actually in the fact, that we tried to derive a relativistic single-particle wave function. Such an endeavour has, however, to fail. Having access to very large energies, we can always have pair creation. If we want to describe single electrons $|e^-\rangle$ interacting with photons, we always will have the possibility of e.g. an electron sending out a photon, which again splits up into an electron-positron pair. Thus the 3 particle state $|e^-e^+e^-\rangle$ has also to be taken into account, as well as states with even more particle. This can only be done in the framework of **Quantum Field Theory**, the topic of one of the Level 4 courses.
We will here , however, follow the historic path, where first another single particle wave function was introduced.

- *To repeat this lecture:* Chapter [15.1] of [1]

- *To prepare for next lecture:* Chapter [15.2] of [1]

12 The Dirac equation

12.1 Introduction

Dirac saw the root of some of the problems of the Klein-Gordon-equation in the fact that this is a second order equation in time. Thus he tried hard to get a first order equation from the relativistic energy-momentum relation and finally succeeded.

Today we know that the correct language for relativistic processes is **quantum field theory** and within this framework the mentioned problems of the Klein-Gordon-equation disappear. Thus we do not have to care a priori whether the wave equations are first or second order. Moreover a system of n second order differential equations can always be written as a system of $2n$ first order equations.

From a modern point of view, we start at looking at the possible **representations** of the **Lorentz group**, to get the **Klein-Gordon-equation** for s=0 particles, the **Dirac-equation** for s=1/2 particle, the **Maxwell-equations** for s = 1 particles (**Proca-equation** for massive s= 1) and the **Rarita-Schwinger-equation** for s = 3/2 particles.

For pedagogical reasons we will follow here, however, the historical route, which led Dirac in 1928 [21] - to some extent by chance - to the right result for the electron, by demanding the wave equation to be of first order in time.

12.2 Derivation

Dirac started from the following first order Ansatz

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = \left(\frac{\hbar c}{i}\alpha^k\partial_k + \beta mc^2\right)\Psi = H\Psi\ .}$$

(319)

This equation should of course fulfil the relativistic energy-momentum relation. To test this requirement we look at $H^2\Psi$:

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = \left(\frac{\hbar c}{i}\alpha^i\partial_i + \beta mc^2\right)\left(\frac{\hbar c}{i}\alpha^j\partial_j + \beta mc^2\right)\Psi \tag{320}$$

$$= \left[-\hbar^2 c^2\alpha^i\alpha^j\partial_i\partial_j + \frac{\hbar mc^3}{i}(\alpha^i\beta + \beta\alpha^i)\partial_i + m^2c^4\beta^2\right]\Psi \tag{321}$$

$$= \left[-\hbar^2 c^2\frac{\alpha^i\alpha^j + \alpha^j\alpha^i}{2}\partial_i\partial_j + \frac{\hbar mc^3}{i}(\alpha^i\beta + \beta\alpha^i)\partial_i + m^2c^4\beta^2\right]\Psi \tag{322}$$

$$\overset{!}{=} \left[-\hbar^2 c^2\delta^{ij}\partial_i\partial_j + m^2c^4\right]\Psi . \tag{323}$$

Thus α^i and β have to fulfil the following conditions

$$\alpha^i\alpha^j + \alpha^j\alpha^i = 2\delta^{ij} , \tag{324}$$

$$\alpha^i\beta + \beta\alpha^i = 0 , \tag{325}$$

$$\beta^2 = 1 . \tag{326}$$

This clearly can not be fulfilled by simple numbers, but matrices might do the job. α_i and β are called **Dirac-matrices**.
The following form of the Dirac- matrices is called **Dirac representation**; it fulfils Eq.(324-326):

$$\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix} , \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} , \tag{327}$$

with the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \qquad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{328}$$

The Pauli matrices have the following properties

$$\left[\sigma^i, \sigma^j\right] = 2i\epsilon^{ijk}\sigma^k , \tag{329}$$

$$\left\{\sigma^i, \sigma^j\right\} = 2\delta^{ij}I_2 . \tag{330}$$

From this we immediately see

$$(\sigma^i)^2 = I_2 , \tag{331}$$

$$\sigma^i\sigma^j = i\epsilon^{ijk}\sigma^k \qquad \text{for } i \neq j , \tag{332}$$

$$\text{Tr}(\sigma^i) = 0 , \tag{333}$$

$$\det(\sigma^i) = -1 . \tag{334}$$

With this definitions Eq.(324-326) can be easily checked.

Remarks:

- I is obvious that the matrices in Eq.(327) are hermitian, i.e.

$$\beta^\dagger = \beta , \qquad \alpha^{k\dagger} = \alpha^k . \tag{335}$$

- The form of the Dirac matrices is not unique! Every non-singular transformation of Eq.(327) $M\alpha^i M^{-1}$, $M\beta M^{-1}$ fulfils also Eq.(324-326).

$$\begin{align}
M\alpha^i M^{-1} M\alpha^j M^{-1} + M\alpha^j M^{-1} M\alpha^i M^{-1} &= 2\delta^{ij} , & (336) \\
M\alpha^i M^{-1} M\beta M^{-1} + M\beta M^{-1} M\alpha^i M^{-1} &= 0 , & (337) \\
M\beta M^{-1} M\beta M^{-1} &= 1 . & (338)
\end{align}$$

Every unitary transformation of Eq.(327) gives again hermitian Dirac matrices.

$$\begin{align}
\left(M\alpha^i M^{-1}\right)^\dagger &= (M^{-1})^\dagger (\alpha^i)^\dagger M^\dagger = M\alpha^i M^{-1} & (339) \\
\Leftrightarrow \quad M^{-1} &= M^\dagger . & (340)
\end{align}$$

- This derivation also implies that the wave function Ψ is now a four component object. It is called the **Dirac-spinor**.

12.3 Continuity equation

One of the motivations for deriving the Dirac-equation was to cure the problem of negative probabilities. Hence we derive here a continuity equation and check whether the probability density is positive definite.

The Dirac spinor Ψ and its adjoint (complex conjugated and transpose) spinor $\Psi^\dagger$ are defined as

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} , \qquad \Psi^\dagger = (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*) . \tag{341}$$

We multiply the Dirac-equation from Eq.(319)b with $\Psi^\dagger$ from the left and get

$$i\hbar \Psi^\dagger \frac{\partial \Psi}{\partial t} = \frac{\hbar c}{i} \Psi^\dagger \alpha^k \partial_k \Psi + mc^2 \Psi^\dagger \beta \Psi . \tag{342}$$

The adjoint relation to that reads

$$-i\hbar \frac{\partial \Psi^\dagger}{\partial t} \Psi = -\frac{\hbar c}{i} \partial_k \Psi^\dagger \alpha^{k\dagger} \Psi + mc^2 \Psi^\dagger \beta^\dagger \Psi \ . \tag{343}$$

The difference of these two equations, Eq.(342) - Eq.(343) - gives

$$i\hbar \frac{\partial}{\partial t} \left(\Psi^\dagger \Psi\right) = \frac{\hbar c}{i} \left(\Psi^\dagger \alpha^k \partial_k \Psi + \partial_k \Psi^\dagger \alpha^{k\dagger} \Psi\right) + mc^2 \left(\Psi^\dagger \beta \Psi - \Psi^\dagger \beta^\dagger \Psi\right) \ . \tag{344}$$

Taking into account that α_k and β are hermitian, i.e. $\alpha_k^\dagger = \alpha_k$ and $\beta^\dagger = \beta$ we get

$$i\hbar \frac{\partial}{\partial t} \left(\Psi^\dagger \Psi\right) = \frac{\hbar c}{i} \partial_k \left(\Psi^\dagger \alpha^k \Psi\right) \tag{345}$$

$$\frac{\partial}{\partial t} \left(\Psi^\dagger \Psi\right) + c\partial_k \left(\Psi^\dagger \alpha^k \Psi\right) = 0 \tag{346}$$

$$\frac{\partial}{\partial t}\rho + \vec{\nabla}\vec{j} = 0 \ . \tag{347}$$

In the last line we defined the probability density ρ to be

$$\rho = \Psi^\dagger \Psi = |\psi_1|^2 + \cdots + |\psi_4|^2 \ , \tag{348}$$

which is obviously positive definite and the current density to be

$$j_k = c\Psi^\dagger \alpha^k \Psi \ . \tag{349}$$

The continuity equation can also be written in a co-variant form

$$\partial_\mu j^\mu = 0 \ , \tag{350}$$

with

$$j^0 := c\rho \ , \tag{351}$$

$$j^\mu := (j^0, j^k) \ . \tag{352}$$

12.4 Co-Variant formulation of Dirac theory

In order to write the Dirac equation in Eq.(319) in a form, where the Lorentz invariance will become more obvious we multiply Eq.(319) with $-\beta/(\hbar c)$ from the right-hand side:

$$-i\beta \frac{\partial \Psi}{\partial ct} + \left(\frac{1}{i}\beta\alpha^k \partial_k + \frac{mc}{\hbar}\right)\Psi = 0 \ . \tag{353}$$

With $\partial_0 = \partial/\partial(ct)$ and the definitions for the γ-**matrices**

$$\gamma^0 := \beta , \tag{354}$$
$$\gamma^k := \beta\alpha^k , \tag{355}$$

this becomes

$$\left(-i\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\Psi = 0 . \tag{356}$$

Remarks:

- Hermiticity: γ^0 is hermitian and γ^k is anti-hermitian.

$$\left(\gamma^0\right)^\dagger = \beta^\dagger = \beta = \gamma^0 , \tag{357}$$
$$\left(\gamma^k\right)^\dagger = \left(\beta\alpha^k\right)^\dagger = (\alpha^k)^\dagger\beta^\dagger = \alpha^k\beta = -\beta\alpha^k = -\gamma^k . \tag{358}$$

- Defining equation for the γ-matrices:

$$(\gamma^0)^2 = (\beta)^2 = 1_2 , \tag{359}$$
$$\left(\gamma^k\right)^2 = \beta\alpha^k\beta\alpha^k = -\beta\beta\alpha^k\alpha^k = -1_2 , \tag{360}$$
$$\gamma^0\gamma^k + \gamma^k\gamma^0 = \beta\beta\alpha^k + \beta\alpha^k\beta = 0 , \tag{361}$$
$$\gamma^k\gamma^l + \gamma^l\gamma^k = \beta\alpha^k\beta\alpha^l + \beta\alpha^l\beta\alpha^k = 0 \ (l \neq k) . \tag{362}$$

This can be written compactly as

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}1_4 . \tag{363}$$

- Co-Variant γ-matrices:
$$\gamma_\mu = g_{\mu\nu}\gamma^\nu . \tag{364}$$

- Different representations of the γ-matrices. Every non-singular transformation of γ^μ fulfils also Eq.(363). Examples are the **Majorana representation** or the **chiral representation**.

Using the so-called **Feynman-slash**, that abbreviates the contraction of an arbitrary four-vector B_μ with the γ-matrices γ^μ

$$\not{B} := B_\mu\gamma^\mu = B^\mu\gamma_\mu = B^0\gamma^0 - \vec{B}\cdot\vec{\gamma} , \tag{365}$$

the Dirac equation becomes now

$$\left(-i\not{\partial} + \frac{mc}{\hbar}\right)\Psi = 0 . \tag{366}$$

Using in addition natural units the Dirac equation becomes very simple

$$\left(-i\slashed{\partial} + m\right)\Psi = 0\ . \tag{367}$$

- *To repeat this lecture:* Chapter [15.2/3] of [1]

- *To prepare for next lecture:* Chapter [15.3] of [1]

13 Lorentz-invariance of the Dirac equation

— Chapter [15.3] of [1] —

13.1 Lorentz transformation

In order to discuss the Lorentz-invariance of the Dirac equation we start by setting our notation. The space-time vectors are given as a **contra-variant vector**

$$x^\mu = \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix} = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} \tag{368}$$

or as a **co-variant vector**

$$x_\mu = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} ct \\ -x \\ -y \\ -z \end{pmatrix} . \tag{369}$$

The metric tensor is given by

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} . \tag{370}$$

This gives the following relations

$$g_{\mu\nu} = g^{\mu\nu} , \tag{371}$$
$$x_\mu = g_{\mu\nu} x^\nu , \tag{372}$$
$$x^\mu = g^{\mu\nu} x_\nu , \tag{373}$$
$$g^\mu_\nu = g^{\mu\sigma} g_{\sigma\nu} = \delta^\mu_\nu . \tag{374}$$

A **Lorentz-transformation**[4] is a transformation between two systems, that move relatively to each other with a constant velocity. The most general form is given by the **inhomogeneous Lorentz-transformation** or **Poincare-transformation**; it reads

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu . \tag{375}$$

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[4]Named after **Hendrik Antoon Lorentz** (1853-1928, NL, NP 1902) - not to confuse with the Lorenz gauge from **Ludvig Lorenz** (1829 -1891, DK). There is also a Lorentz-Lorenz equation in the literature...

These transformations consist of translations (a^μ) and the **homogeneous Lorentz-transformations** ($\Lambda^\mu{}_\nu$), which can again be split up in **Rotations** (in space), **Lorentz-boosts** and some discrete transformations like **parity** (space-reflection) or **time-reflection**[5]

Remarks:

- The differential operator transforms as

$$\partial_\mu \; = \; \frac{\partial}{\partial x^\mu} = \frac{\partial x^{\nu'}}{\partial x^\mu}\frac{\partial}{\partial x^{\nu'}} \tag{376}$$

$$= \; \Lambda^\nu{}_\mu \frac{\partial}{\partial x^{\nu'}} = \Lambda^\nu{}_\mu \partial_{\nu'} \; . \tag{377}$$

  It has the same transformation property as x_μ.

- Every 4-component object that transforms as given in Eq.(375), is called a **4-vector**. Examples are x^μ and ∂^μ, the four-momentum p^μ and the vector potential A^μ. Scalar products of four-momenta have the same value in all systems!

- The D'Alembert operator has to be invariant under Lorentz-transformations

$$\Box \; = \; \partial_\mu \partial^\mu = \partial_\mu g^{\mu\nu} \partial_\nu \tag{378}$$

$$= \; \Lambda^\alpha{}_\mu g^{\mu\nu} \Lambda^\beta{}_\nu \partial_{\alpha'} \partial_{\beta'} \tag{379}$$

$$\overset{!}{=} \; g^{\alpha\beta} \partial_{\alpha'} \partial_{\beta'} \; , \tag{380}$$

  which gives the relation

$$\Lambda^\alpha{}_\mu g^{\mu\nu} \Lambda^\beta{}_\nu = g^{\alpha\beta} \Leftrightarrow \Lambda g \Lambda^t = g \; . \tag{381}$$

  The last equation actually defines the homogeneous Lorentz group and it gives

$$\det\Lambda \; = \; \pm 1 \; , \tag{382}$$

$$\Lambda^0{}_0 \; \geq \; 1 \;\; \text{or} \;\; \Lambda^0{}_0 \leq 1 \; . \tag{383}$$

The **proper Lorentz-transformations** are defined by $\det\Lambda = +1$ and $\Lambda^0{}_0 \geq 1$. They consist of rotations of the three-dimensional space

---

[5]An investigation of such a symmetry might sound to be a very academic exercise, but it actually turns out that the study of this symmetry and its violations is crucial to understand the existence of matter in the universe, see e.g. [22].

and of Lorentz-boosts.

An example for a space rotation is e.g.

$$
R_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\phi & \sin\phi & 0 \\ 0 & -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} , \tag{384}
$$

an example for a Lorentz-boost is e.g.

$$
L_{01} = \begin{pmatrix} \cosh\eta & -\sinh\eta & 0 & 0 \\ -\sinh\eta & \cosh\eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{1-\beta^2}} & \frac{-\beta}{\sqrt{1-\beta^2}} & 0 & 0 \\ \frac{-\beta}{\sqrt{1-\beta^2}} & \frac{1}{\sqrt{1-\beta^2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} ,
$$
$$\tag{385}$$

with $\beta = v/c$ and $\tanh\eta = \beta$. The representation of the full Lorentz-group is described in detail in [5].

13.2   Lorentz invariance of the Dirac equation

Now we want to see how the Dirac equation transforms when performing a Lorentz-transformation. We consider two systems:

System I :	Coordinate x^μ	spinor Ψ
System I' :	Coordinate $x^{\mu'}$	spinor Ψ'

$$\tag{386}$$

The transformations from I to I' read

$$
x' = \Lambda x + a , \tag{387}
$$
$$
\Psi'(x') = S(\Lambda)\Psi(x) , \tag{388}
$$

with an unknown transformation $S(\Lambda)$.

Starting from the Dirac equation in System I

$$
\left(-i\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\Psi(x) = 0 , \tag{389}
$$

we transform ∂_μ and $\Psi(x)$ into the system I'

$$
\partial_\mu = \Lambda^\nu{}_\mu\partial'_\nu , \tag{390}
$$
$$
\Psi(x) = S(\Lambda)^{-1}\Psi'(x') , \tag{391}
$$

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to get

$$\left(-i\gamma^\mu\Lambda^\nu{}_\mu\partial'_\nu + \frac{mc}{\hbar}\right)S(\Lambda)^{-1}\Psi'(x') = 0 \tag{392}$$

$$\left(-iS(\Lambda)\gamma^\mu\Lambda^\nu{}_\mu S(\Lambda)^{-1}\partial'_\nu + \frac{mc}{\hbar}\right)\Psi'(x') = 0 \, . \tag{393}$$

In the second line we have multiplied everything with $S(\Lambda)$ from the r.h.s. .
The Dirac equation is now form invariant, if

$$S(\Lambda)\gamma^\mu\Lambda^\nu{}_\mu S(\Lambda)^{-1} = \gamma^\nu \tag{394}$$

$$\Leftrightarrow \gamma^\mu\Lambda^\nu{}_\mu = S(\Lambda)^{-1}\gamma^\nu S(\Lambda) \, . \tag{395}$$

Remarks:

- Any four component that transforms as given by Eq.(388) is called a **Dirac-spinor**.

- The transformation matrix S is defined by Eq.(395).

- A detailed construction of S is described in detail e.g. in [5]. Here two examples.

  1. A space rotation around the z-axis:

  $$R_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\phi & \sin\phi & 0 \\ 0 & -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

  $$\Rightarrow S_{R_{12}} = \begin{pmatrix} \cos\frac{\phi}{2} + i\sin\frac{\phi}{2} & 0 & 0 & 0 \\ 0 & \cos\frac{\phi}{2} - i\sin\frac{\phi}{2} & 0 & 0 \\ 0 & 0 & \cos\frac{\phi}{2} + i\sin\frac{\phi}{2} & 0 \\ 0 & 0 & 0 & \cos\frac{\phi}{2} - i\sin\frac{\phi}{2} \end{pmatrix} \, . \tag{396}$$

  Note that the matrix R_{12} has a periodicity of 2π, while $S_{R_{12}}$ has a periodicity of 4π.

  2. A Lorentz-boost along the x-axis

  $$L_{01} = \begin{pmatrix} \cosh\eta & -\sinh\eta & 0 & 0 \\ -\sinh\eta & \cosh\eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

  $$\Rightarrow S_{L_{01}} = \begin{pmatrix} \cosh\frac{\eta}{2} & 0 & 0 & \sinh\frac{\eta}{2} \\ 0 & \cosh\frac{\eta}{2} & \sinh\frac{\eta}{2} & 0 \\ 0 & \sinh\frac{\eta}{2} & \cosh\frac{\eta}{2} & 0 \\ \sinh\frac{\eta}{2} & 0 & 0 & \cosh\frac{\eta}{2} \end{pmatrix} \, . \tag{397}$$

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13.3   Bilinear forms

The **adjoint spinor** is defined as

$$\bar{\Psi} = \Psi^\dagger \gamma^0 \ . \tag{398}$$

It transforms as

$$\Psi' = S\Psi \quad \Rightarrow \quad \Psi'^\dagger = \Psi^\dagger S^\dagger \tag{399}$$

$$\Rightarrow \quad \bar{\Psi}' = \Psi^\dagger S^\dagger \gamma^0 \ . \tag{400}$$

One can show (e.g. [5]) that

$$S^\dagger \gamma^0 = b\gamma^0 S^{-1} \ , \tag{401}$$

with

$$b = \begin{cases} +1 & \text{for} \quad \Lambda^{00} \geq +1 \\ -1 & \text{for} \quad \Lambda^{00} \leq -1 \end{cases} \ . \tag{402}$$

Thus we get for the transformation of the adjoint spinor

$$\bar{\Psi}' = \bar{\Psi} S^{-1} \ , \tag{403}$$

if we only consider transformations that do not change the direction of time. Now we can derive the transformation properties of the following bilinears

$$
\begin{array}{ccccccc}
\bar{\Psi}' & & \Psi' & = & & \bar{\Psi} & & \Psi \ , \\
\bar{\Psi}' & \gamma^\mu & \Psi' & = & \Lambda^\mu{}_\alpha & \bar{\Psi} & \gamma^\alpha & \Psi \ , \\
\bar{\Psi}' & \sigma^{\mu\nu} & \Psi' & = & \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta & \bar{\Psi} & \sigma^{\alpha\beta} & \Psi \ ,
\end{array}
\tag{404}
$$

with

$$\sigma^{\mu\nu} := \frac{i}{2} \left[\gamma^\mu, \gamma^\nu \right] \ . \tag{405}$$

Thus we get the following transformation properties

1. $\bar{\Psi}\Psi$ transforms as a **Lorentz-scalar**.

2. $\bar{\Psi}\gamma^\mu\Psi$ transforms as a **Lorentz-vector**. γ^μ alone is not a Lorentz-vector! It is always given by the Definition in Eq.(363).

3. $\bar{\Psi}\sigma^{\mu\nu}\Psi$ transforms as a **Lorentz-tensor**.

- *To repeat this lecture:* Chapter [15.3] of [1]

- *To prepare for next lecture:* Chapter [15.4/6] of [1]

14 Solutions of the Dirac equation

14.1 Plane wave solutions of the Dirac equation

We are looking now for solutions of the free Dirac equation of the form

$$\Psi(\vec{r}, t) = A \cdot u \cdot e^{i\frac{\vec{p} \cdot \vec{r} - Et}{\hbar}} = A \cdot u \cdot e^{-i\frac{p_\mu x^\mu}{\hbar}} . \tag{406}$$

A is a constant, u is a four component spinor being independent from the space-time coordinate x_μ. Inserting this ansatz into Eq.(319) we get

$$Eu = \left(c\alpha^k p_k + \beta mc^2\right) u . \tag{407}$$

To get a first idea about the structure of this solution we consider the case of a particle at rest, i.e. $\vec{p} = 0$. We get

$$Eu(0) = mc^2 \beta u(0) = \begin{pmatrix} mc^2 I_2 & 0 \\ 0 & -mc^2 I_2 \end{pmatrix} u(0) . \tag{408}$$

This equation has two different eigenvalues $E_+ = +mc^2$ and $E_- = -mc^2$, that occur each twice and the following four eigenvectors

$$u^{(1)}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \quad u^{(2)}(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} , \quad u^{(3)}(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} , \quad u^{(4)}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} . \tag{409}$$

The first two spinors describe a spin $1/2$ particle and the second two a spin $1/2$ anti-particle.

The positron, the anti-particle of the electron was discovered in 1932, about 4 years afterwards the Dirac-equation was postulated. This created also a whole new field of science-fiction literature, see e.g. [23].

If we have a solution of the form $c_1 u^{(1)}(0) + c_2 u^{(2)}(0) + c_3 u^{(3)}(0) + c_4 u^{(4)}(0)$ in the system, where the particle is at rest $\vec{p} = 0$, then we get in the system that has a finite momentum $\vec{p'}$ in x-direction

$$\Psi'(\vec{r'}, t') = A \cdot u' \cdot e^{i\frac{\vec{p'} \cdot \vec{r'} - E't'}{\hbar}} = A \cdot u' \cdot e^{-i\frac{p'_\mu x^{\mu'}}{\hbar}} , \tag{410}$$

with

$$u' = Su = c_1 \begin{pmatrix} \cosh\frac{\eta}{2} \\ 0 \\ 0 \\ \sinh\frac{\eta}{2} \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ \cosh\frac{\eta}{2} \\ \sinh\frac{\eta}{2} \\ 0 \end{pmatrix} + c_3 \begin{pmatrix} 0 \\ \sinh\frac{\eta}{2} \\ \cosh\frac{\eta}{2} \\ 0 \end{pmatrix} + c_4 \begin{pmatrix} \sinh\frac{\eta}{2} \\ 0 \\ 0 \\ \cosh\frac{\eta}{2} \end{pmatrix} . \tag{411}$$

14.2 Non-relativistic limit of the Dirac-equation

To discuss the non-relativistic limit of the Dirac equation we start from the free Dirac-equation and couple the electro-magnetic field via minimal coupling.

$$i\hbar\frac{\partial \Psi}{\partial t} = \left[c\alpha^k\left(p_k - \frac{e}{c}A_k\right) + \beta mc^2 + e\Phi\right]\Psi. \tag{412}$$

Next we decompose the four-component Dirac-spinor Ψ into two two-component spinors $\tilde{\phi}$ and $\tilde{\chi}$.

$$\Psi = \left(\begin{array}{c} \tilde{\phi} \\ \tilde{\chi} \end{array}\right) \tag{413}$$

Inserting this into Eq.(412) we get

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c} \tilde{\phi} \\ \tilde{\chi} \end{array}\right) = c\left(\begin{array}{c} \vec{\sigma}\cdot\vec{\pi}\tilde{\chi} \\ \vec{\sigma}\cdot\vec{\pi}\tilde{\phi} \end{array}\right) + e\Phi\left(\begin{array}{c} \tilde{\phi} \\ \tilde{\chi} \end{array}\right) + mc^2\left(\begin{array}{c} \tilde{\phi} \\ -\tilde{\chi} \end{array}\right), \tag{414}$$

with the operator of the canonical momentum

$$\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}. \tag{415}$$

In order to investigate the non-relativistic limit, we first split of the dominant energy dependence, which is given by mc^2. We define

$$\left(\begin{array}{c} \tilde{\phi} \\ \tilde{\chi} \end{array}\right) =: e^{-\frac{imc^2}{\hbar}t}\left(\begin{array}{c} \phi \\ \chi \end{array}\right). \tag{416}$$

In the non-relativistic limit the remaining time-dependence of ϕ and χ will be much weaker than the explicit exponential term. Then we get

$$i\hbar\frac{\partial}{\partial t}\left(\begin{array}{c} \phi \\ \chi \end{array}\right) = c\left(\begin{array}{c} \vec{\sigma}\cdot\vec{\pi}\chi \\ \vec{\sigma}\cdot\vec{\pi}\phi \end{array}\right) + e\Phi\left(\begin{array}{c} \phi \\ \chi \end{array}\right) - 2mc^2\left(\begin{array}{c} 0 \\ \chi \end{array}\right). \tag{417}$$

Next we make in the second line of the equation above the following assumption

$$i\hbar\partial_t\chi, e\Phi\chi \ll 2mc^2\chi \tag{418}$$

to get

$$\chi = \frac{\vec{\sigma}\cdot\vec{\pi}}{2mc}\phi = \mathcal{O}\left(\frac{v}{c}\right)\phi. \tag{419}$$

Thus ϕ is denoted the large component of the Dirac-spinor and χ as the small component. Next we insert Eq.(419) into the first line of Eq.(417) and we get

$$i\hbar\frac{\partial \phi}{\partial t} = \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{\pi}) + e\Phi\right]\phi. \tag{420}$$

Using the identity

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot (\vec{a} \times \vec{b}) , \tag{421}$$

one gets

$$(\vec{\sigma} \cdot \vec{\pi})(\vec{\sigma} \cdot \vec{\pi}) = \pi^2 + i\vec{\sigma} \cdot (\vec{\pi} \times \vec{\pi}) \tag{422}$$

$$= \pi^2 - \frac{e\hbar}{c}\vec{\sigma} \cdot \vec{B} . \tag{423}$$

So we get for the large component

$$i\hbar\frac{\partial \phi}{\partial t} = \left[\frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{e\hbar}{2mc}\vec{\sigma} \cdot \vec{B} + e\Phi \right] \phi . \tag{424}$$

This is the **Pauli-equation** that describes non-relativistic electrons with spin 1/2. Moreover the Dirac equation gives automatically the correct Lande factor $g = 2$ of the electron, which had to be introduced by hand to the Pauli-equation in order to be compatible with experiment. We can introduce the Lande factor in the above equation via $\vec{\sigma} \to g\vec{\sigma}/2$.

Looking at the special case of a constant $\vec{B}$-field

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{x} , \tag{425}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} , \tag{426}$$

we arrive at

$$i\hbar\frac{\partial \phi}{\partial t} = \left[\frac{\vec{p}^2}{2m} - \frac{e}{2mc}(\vec{L} + 2\vec{S}) \cdot \vec{B} + \frac{e^2}{2mc^2}\vec{A}^2 + e\Phi \right] \phi , \tag{427}$$

with $\vec{S} = \hbar\vec{\sigma}/2$ and $\vec{L} = \vec{x} \times \vec{p}$. The factor 2 in front of $\vec{S}$ in Eq.(427) represents the Lande factor g.

More precise measurements have shown, however, that the Lande-factor deviates slightly from 2, thus the anomalous magnetic moment of the electron is introduced as

$$a = \frac{g - 2}{2} . \tag{428}$$

This quantity is measured very precisely by now. Theoretical deviations from the prediction of the Dirac equation ($a = 0$) arise as soon as one is considering the effects of Quantum electro dynamics (QED). The most precise values are currently [24, 25]

$$a^{Exp.} = 0.00115965218073(28) , \tag{429}$$

$$a^{Theo.} = 0.00115965218178(77) . \tag{430}$$

This is an amazing agreement! This is the most precise tested prediction in science.

To reach this, accuracy 12672 5-loop diagrams have to be calculated [25] in QED.
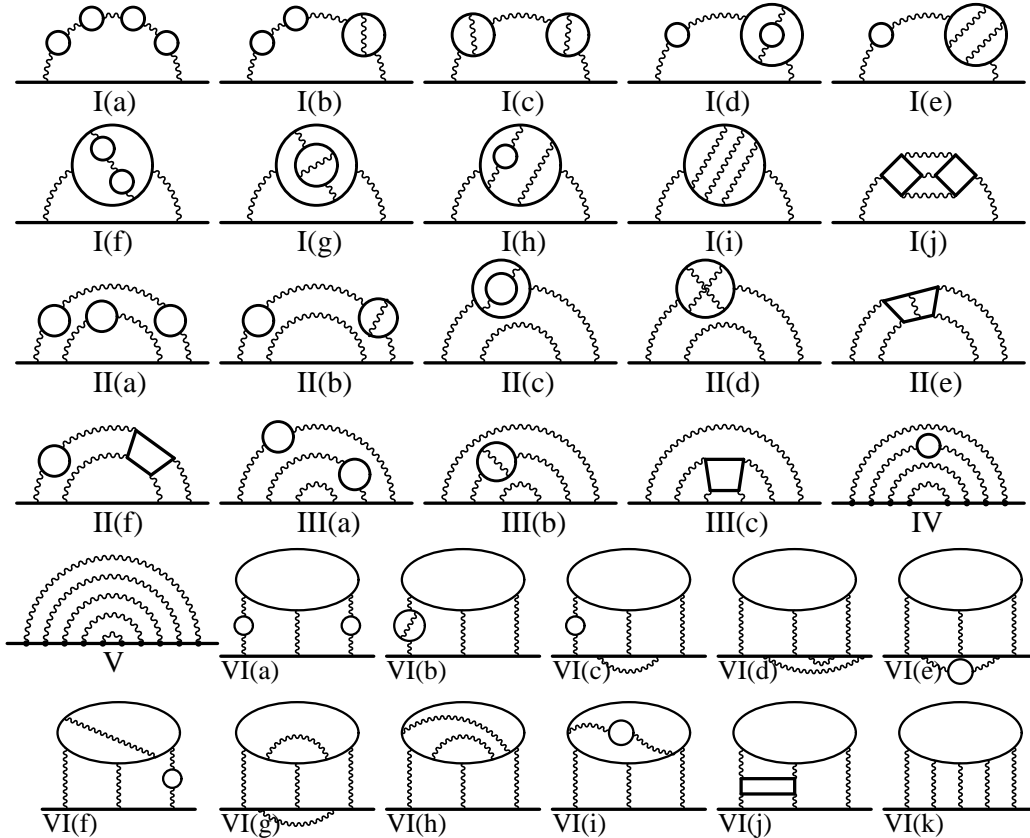
Nowadays the above comparison is used to fix the numerical value of the electro-magnetic coupling, $\alpha_e = e^2/(4\pi)$.

Short excursion: Quantum electro dynamics (QED)

- Classical mechanics can be described by Newton's law

$$\vec{F} = m\frac{d^2}{dt^2}\vec{x} \ . \tag{431}$$

Some problems can, however, be solved much easier if one starts from the Lagrange function L, defined as the difference between kinetic and potential energy

$$L = T - V \ . \tag{432}$$

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Newton's law can be derived from the Lagrange function via the Euler-Lagrange equations.

- Similarly free relativistic electrons can be described by the Dirac equation

$$\left(i\partial\!\!\!/ - m\right)\Psi = 0 \ ,\tag{433}$$

  while it is many times advantageous to use instead a Lagrangian density given by

$$\mathcal{L} = \bar{\Psi}\left(i\partial\!\!\!/ - m\right)\Psi \ .\tag{434}$$

  Here again the Dirac equation can be derived from the Lagrange density via generalisations of the Euler-Lagrange equations.

- Finally the free Maxwell-equations

$$\partial_\mu F^{\mu\nu} = 0\tag{435}$$

  are equivalent to the following Lagrange density

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} \ .\tag{436}$$

- Combining free electrons with free photons one gets thus

$$\mathcal{L} = \bar{\Psi}\left(i\partial\!\!\!/ - m\right)\Psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \ .\tag{437}$$

- Interaction between electrons and photons can again be switched on via minimal coupling, this is equivalent to the following replacement

$$\partial_\mu \to D_\mu = \partial_\mu - ieA_\mu\tag{438}$$

  to obtain the complete Lagrangian of QED

$$\mathcal{L} = \bar{\Psi}\left(i D\!\!\!\!/ - m\right)\Psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \ .\tag{439}$$

  Remarks:

  - All terms in the QED Lagrangian are Lorentz-scalars!
  - The interaction term looks like $e\bar{\Psi}A\!\!\!/\Psi$.

- *To repeat this lecture:* Chapter [15.4] of [1]

- *To prepare for next lecture:* Chapter [15.5] of [1]

15 Solutions of the Dirac equation for a central potential

For the case of a central potential the Dirac-equation reads

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \left[c\alpha^k p_k + \beta mc^2 + e\Phi\right]\Psi(\vec{r},t) . \tag{440}$$

With $e\Phi = V(r)$ and the ansatz $\Psi(\vec{r},t) = e^{-i\frac{E}{\hbar}t}\Psi(\vec{r})$ this becomes

$$E\Psi(\vec{r}) = \left[c\alpha^k p_k + \beta mc^2 + V(r)\right]\Psi(\vec{r}) . \tag{441}$$

Next we would like to separate the variables as in the case of the Schrödinger-equation. There we had $\vec{L}^2$ and L_z as conserved quantum numbers and we found solutions that are simultaneous eigenvectors of H, $\vec{L}^2$ and L_z. Since the Dirac-equation always contains spin, we expect now that not the angular momentum $\vec{L}$ is conserved, but the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. An explicit calculation gives

$$[H, \vec{L}] = -i\hbar c(\vec{\alpha}\times\vec{p}) \neq 0 , \tag{442}$$

proofing that the angular momentum is not conserved.
The **spin operator** is given by

$$\vec{S} = \frac{\hbar}{2}\vec{\Sigma} , \tag{443}$$

with

$$\Sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix} . \tag{444}$$

Remarks: this definition gives

- The angular momentum commutation relation is fulfilled

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k . \tag{445}$$

- The eigenvalues of $\vec{S}^2$ read

$$\vec{S}^2\Psi = \frac{3}{4}\hbar^2\Psi = s(s+1)\hbar^2\Psi , \tag{446}$$

with $s = 1/2$.

- The commutator of the spin operator with the Hamiltonian reads

$$[H, \vec{S}] = +i\hbar c(\vec{\alpha} \times \vec{p}) \neq 0 . \tag{447}$$

Comparing Eq.(442) with Eq.(447) we get the conservation of the total angular momentum

$$[H, \vec{J}] = 0 . \tag{448}$$

One can also show that

$$[H, \vec{J}^2] = 0 . \tag{449}$$

Thus we can find wave functions that are simultaneous eigenfunctions of H, $\vec{J}^2$ and J_z, with the eigenvalues E, $j(j+1)\hbar^2$ and $m_j\hbar$.

We make the following ansatz for the Dirac-equation with a spherical potential

$$\Psi^l_{jm_j}(r, \theta, \phi) = \begin{pmatrix} \frac{iG_{lj}(r)}{r} & \phi^l_{jm_j}(\theta, \phi) \\ \frac{iF_{lj}(r)}{r} & (\vec{\sigma} \cdot \frac{\vec{x}}{x}) \; \phi^l_{jm_j}(\theta, \phi) \end{pmatrix} \tag{450}$$

with the 2-component spinors

$$\phi^l_{jm_j}(\theta, \phi) = \begin{cases} \phi^{(+)}_{jm_j}(\theta, \phi) & \text{for} \quad j = l + \frac{1}{2} \\ \phi^{(-)}_{jm_j}(\theta, \phi) & \text{for} \quad j = l - \frac{1}{2} \end{cases} \tag{451}$$

and

$$\phi^{(+)}_{jm_j}(\theta, \phi) = \begin{pmatrix} \sqrt{\frac{l+m_j+\frac{1}{2}}{2l+1}} Y_{l,m_j-\frac{1}{2}}(\theta, \phi) \\ \sqrt{\frac{l-m_j+\frac{1}{2}}{2l+1}} Y_{l,m_j+\frac{1}{2}}(\theta, \phi) \end{pmatrix} , \tag{452}$$

$$\phi^{(-)}_{jm_j}(\theta, \phi) = \begin{pmatrix} \sqrt{\frac{l-m_j+\frac{1}{2}}{2l+1}} Y_{l,m_j-\frac{1}{2}}(\theta, \phi) \\ -\sqrt{\frac{l+m_j+\frac{1}{2}}{2l+1}} Y_{l,m_j+\frac{1}{2}}(\theta, \phi) \end{pmatrix} . \tag{453}$$

Y are the spherical harmonics and $G_{lj}(r)$ and $F_{lj}(r)$ are some unknown functions that describe the radial dependence. They obey the following differential equation

$$\frac{E - m - V(r)}{\hbar c} G_{lj}(r) = -\frac{dF_{lj}(r)}{dr} \mp \left(j + \frac{1}{2}\right) \frac{F_{lj}(r)}{r} \tag{454}$$

$$\frac{E + m - V(r)}{\hbar c} F_{lj}(r) = +\frac{dG_{lj}(r)}{dr} \mp \left(j + \frac{1}{2}\right) \frac{G_{lj}(r)}{r} \tag{455}$$

for $j = l \pm 1/2$. The radial equation are solved by the ansatz

$$F(r) = f(r)e^{-r} =: r^s [a_0 + a_1 r + \ldots] e^{-r} , \tag{456}$$

$$G(r) = g(r)e^{-r} =: r^s [b_0 + b_1 r + \ldots] e^{-r} . \tag{457}$$

In the case a hydrogen-like problem we have $V(r) = -Z\alpha/r$, with $\alpha = e^2/(4\pi\epsilon_0 \hbar c) = 1/137$ and we get then the following energy eigenvalues

$$E_{n,j} = \frac{mc^2}{\sqrt{1 + \left(\dfrac{Z\alpha}{n - \left(j + \frac{1}{2}\right) + \sqrt{\left(j + \frac{1}{2}\right)^2 - (Z\alpha)^2}}\right)^2}} \,, \quad (458)$$

with $\alpha = e^2/(4\pi\epsilon_0 \hbar c)$. Expanding this in $(Z\alpha)$ we get

$$E_{n,j} = mc^2 \left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n}\right) + \mathcal{O}\left(Z^6\alpha^6\right)\right] . \quad (459)$$

The first term is just the rest mass, the second term is the result of the Schrödinger theory for the hydrogen atom and the third term is the first relativistic correction, that gives a fine structure splitting.
More details of this calculation can be found in [5].

- *To repeat this lecture:* Chapter [15.5] of [1]

- *To prepare for next lecture:* Chapter [17.1-4] of [1]

16 Measurements and interpretation

— Chapter [17.1-4] of [1] —

16.1 Introduction

Quantum mechanics is one of the most successful concepts of physics. It is the foundation of many technical applications like Computer, Laser,... The theory is thoroughly tested by experiments and all the predictions agree perfectly with the measurements. In that sense **there is no doubt that quantum mechanics is the correct language to describe microscopic effects**, at least in the energy range, that is currently accessible to us.
The *inherent statistical nature* of quantum mechanical predictions as well as the quantum mechanical concept of *measurements* has, however, always raised fundamental questions about the *interpretation* of the theory. To some extend this is a *philosophical* question, depending also strongly on the definition of the meaning of the word **understanding**. Nevertheless, we would like to conclude this lecture course with a brief overview of different interpretations of quantum mechanics.
Some reviews of this topic can also be found e.g. in [26, 27, 28].

16.2 The basic question

According to what we learnt in the course, the predictions of quantum mechanics have an inherent probabilistic nature. One arising question is now, if this probabilistic nature is a *real* feature of nature or just a failure of our current mathematical formulation. A related question is: what is the nature of the measurement process in quantum mechanics?

Let us start by recapitulating the basics of quantum mechanics:

1. Observables are described by hermitian operators.

   - An observable A is related to a hermitian operator $\hat{A}$.

   - There is a complete set of eigenstates $|n\rangle$ with

$$\hat{A}|n\rangle = a_n|n\rangle \ . \tag{460}$$

   - The real numbers a_n are the possible outcomes of a measurement of the observable A.

2. States, particles,... are described by wave functions (states vectors). A general wave function Ψ can be written as a linear combination of the $|n\rangle$:

$$\Psi = \sum_n c_n |n\rangle \ . \tag{461}$$

3. The time evolution of the system is given by the Schrödinger-equation, the Dirac-equation, the Klein-Gordon-equation...

4. The probability of finding Ψ in the state $|n\rangle$ is given by $|c_n|^2$. The average value of the observable A is given by

$$\langle \hat{A} \rangle \ = \ \langle \Psi | \hat{A} | \Psi \rangle = \sum_n |c_n|^2 a_n \ . \tag{462}$$

5. If we measure the observable A in a system described by Ψ and we get the result a_n then the wave function **collapses** to the state $|n\rangle$.

Here two concepts arise, that are not obvious to understand: the inherent probabilistic nature of quantum mechanics (point 4) and the nature of the measurements (point 5), or in other words: what is actually the collapse of the wave function?

To become more concrete, let us assume that our concern is to measure the position of a particle.

- Quantum mechanics gives us only the probability for finding the particle at a certain location. The probability of finding the particle at time t_0 at the location $\vec{x}_0$ is given by $|\Psi(\vec{x} = \vec{x}_0, t = t_0)|^2$.

- To get a definite answer, we have to measure the position. Let us assume now, that the measurement of the position at time t_0 gave the result $\vec{x}_0$. This means that the original wave function collapsed into a position eigenstate with the eigenvalue $\vec{x}_0$.

Now we know for sure that the particle was at the time t_0 at the position $\vec{x}_0$ and we can ask ourselves next: where was the particle slightly before the measurement?[6] This question is not governed by our general rules of quantum mechanics, some possible answers are [7]:

1. at point $\vec{x}_0$ (realistic position);

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[6]The question, where the particle is slightly afterwards, is trivial. Because of the collapse it is still at $\vec{x}_0$. With time the collapsed wave function will, however, smear out again.

2. nowhere (orthodox position);

3. there is no answer to this question (agnostic position),

Remarks:

1. If the particle was actually at the position $\vec{x}_0$ and we just cannot describe this with quantum mechanics, then this is a kind a failure of the current formulation. In that case there will be a more fundamental theory, that contains all the results from quantum mechanics and in addition knows, where the particle was before the measurement.
   This was e.g. the position of Albert Einstein.
   Since such a new theory is expected to contain more variables, they are also called **hidden variable theories**. They were e.g. investigated by Bohm [29, 30].
   How does the fundamental theory look like?

2. This is somehow the basis of the famous and widespread **Copenhagen interpretation**, that was started by Max Born and worked out e.g. by Niels Bohr. The particle simply did not have the property of having a position before the actual measurement. The measurement itself forced the particle to *go* into a certain position, by the collapse of the wave function
   What is actually the measurement process? What is the collapse of the wave function?

3. This is a practical attitude. We can not answer this hypothetical question, because the only way to answer it, would be to perform a measurement at time $t_0 - \delta t$ and then we still do not know what happened before that measurement. We have no access to information without doing a measurement.
   Don't worry, be happy.

16.3   Einstein-Podolsky-Rosen paradox

The aim of the paper of Einstein, Podolsky and Rosen [31] from 1935, was to prove that the realistic position is the correct one.
To see their argument, consider the decay of a neutral pion (spin = 0) at time t_0 into an electron and a positron (each spin 1/2) [7]

$$\pi^0 \to e^+ + e^- \ . \tag{463}$$

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[7]This example actually stems from [32].

If the pion is at rest then the electron-positron pair is described by the following wave function (spin $= 0$)

$$\frac{1}{\sqrt{2}} \left(| \uparrow\downarrow \rangle - | \downarrow\uparrow \rangle \right) . \tag{464}$$

Next we assume that in some distance x_e of the former position of the pion, the spin of the electron will be measured at the time $t_e > t_0$.

Let us assume that the outcome is spin-up. Thus it is clear that any future measurement of the spin of the positron will give spin-down.

How can this be interpreted?

1. According to the realistic interpretation, the spin of the electron, was always (starting from t_0 on) up and the spin of the positron was always down. This fact was just unknown to us, because we do not know the full theory.

2. According to the orthodox interpretation we have:

$t_0 < t < t_e$ The electron-positron state is completely described by the superposition given in Eq.(464).

$t = t_e$ The wave function collapses.

$t > t_e$ The electron and positron are in pure spin states.

<u>Remarks:</u>

- Somehow it seems that the information about the collapse of the wave function is transported at the time t_e instantly from the location x_e to the position of the positron. Einstein and friends considered this to be obviously impossible, because this would violate **locality** (*"spukhafte Fernwirkung"* $\approx$ *"ghost-like long-distance action"*.

- Thus people were seriously looking for extensions of quantum mechanics that include hidden variables, see e.g. the models of Bohm [29, 30] from 1951.

- A very fundamental and crucial point here is the **entangled** stated given in Eq.(464). Schrödinger coined the name **verschränkte Zustände = entangled states**.

- But actually there is no real information transported, so the issue is still not settled.

16.4 Bell's equation

In 1964 Bell [33] was generalising the above experiment and has shown that there is a measurable difference between position 1 and 2 (this excludes by definition position 3). In addition he pointed out severe problems of theories with hidden variables, giving thus evidence for the orthodox position, albeit locality has to be given up to some extent and we are still left with a lack of understanding of the measurement process.

We take the same experimental setup as in the EPR case, with the generalisation that now the spin-detectors can be moved in arbitrary directions. In the EPR case both were measuring the z-component of the spin, while the electron-spin component is measured relative to the vector $\vec{a}$ and the positron-spin component is measured relative to the vector $\vec{b}$. In the end the relevant observable will be the quantum mechanical average of the product of the two spins $P(\vec{a}, \vec{b})$. The case $\vec{a} = \vec{b}$ gives the result of the EPR-case. In the EPR case quantum mechanics told us that the product will always give $-1 \cdot 1$. Thus we have

$$P(\vec{a}, \vec{a}) = -1 \ . \tag{465}$$

If the vectors are anti-parallel $\vec{a} = -\vec{b}$, we will obviously get

$$P(\vec{a}, -\vec{a}) = +1 \ . \tag{466}$$

For a general direction of the vectors quantum mechanics will give

$$P(\vec{a}, \vec{b}) = -\vec{a} \cdot \vec{b} \ . \tag{467}$$

It will turn out, however, that this simple result is incompatible with theories with hidden variables. To show that, we consider very general models with hidden variables, assuming only that reality is given by the quantum mechanical wave function Ψ and some hidden variable λ.

- $A(\vec{a}, \lambda)$ gives the result of the measurement of the electron spin relative to the vector $\vec{a}$. It can take the values ± 1.

- $B(\vec{b}, \lambda)$ gives the result of the measurement of the positron spin relative to the vector $\vec{b}$. It can take the values ± 1.

If $\vec{a} = \vec{b}$, we have

$$A(\vec{a}, \lambda) = -B(\vec{a}, \lambda) \ . \tag{468}$$

The average of the product of the two measurements is given by

$$P(\vec{a}, \vec{b}) = \int \rho(\lambda) A(\vec{a}, \lambda) B(\vec{b}, \lambda) d\lambda \ , \tag{469}$$

with $\rho(\lambda)$ being the unknown probability distribution of the hidden variable. We only demand

$$0 \leq \rho(\lambda) \quad \leq \quad 1 \,, \tag{470}$$

$$\int \rho(\lambda) d\lambda \quad = \quad 1 \,. \tag{471}$$

Because of $B(\vec{b}, \lambda) = -A(\vec{b}, \lambda)$ we get

$$P(\vec{a}, \vec{b}) = -\int \rho(\lambda) A(\vec{a}, \lambda) A(\vec{b}, \lambda) d\lambda \,. \tag{472}$$

Next we take an additional general unit vector $\vec{c}$ to get

$$P(\vec{a}, \vec{b}) - P(\vec{a}, \vec{c}) \quad = \quad -\int \rho(\lambda) \left[A(\vec{a}, \lambda) A(\vec{b}, \lambda) - A(\vec{a}, \lambda) A(\vec{c}, \lambda) \right] d\lambda \tag{473}$$

$$= \quad -\int \rho(\lambda) \left[|A(\vec{b}, \lambda)|^2 A(\vec{a}, \lambda) A(\vec{b}, \lambda) - |A(\vec{b}, \lambda)|^2 A(\vec{a}, \lambda) A(\vec{c}, \lambda) \right] d\lambda \tag{474}$$

$$= \quad -\int \rho(\lambda) \left[1 - A(\vec{b}, \lambda) A(\vec{c}, \lambda) \right] A(\vec{a}, \lambda) A(\vec{b}, \lambda) d\lambda \,. \tag{475}$$

Here we used $|A(\vec{b}, \lambda)|^2 = 1$. Next we keep in mind

$$\rho(\lambda) \left[1 - A(\vec{b}, \lambda) A(\vec{c}, \lambda) \right] \quad \geq \quad 0 \,, \tag{476}$$

$$-1 \leq A(\vec{a}, \lambda) A(\vec{b}, \lambda) \quad \leq \quad +1 \,, \tag{477}$$

to get

$$|P(\vec{a}, \vec{b}) - P(\vec{a}, \vec{c})| \quad \leq \quad \int \rho(\lambda) \left[1 - A(\vec{b}, \lambda) A(\vec{c}, \lambda) \right] d\lambda \tag{478}$$

$$= \quad 1 + P(\vec{b}, \vec{c}) \,. \tag{479}$$

This is the famous **unequality of Bell**.
Combing this with the quantum mechanical result for $P(\vec{a}, \vec{b})$ we get

$$|\vec{a} \cdot \vec{b} - \vec{a} \cdot \vec{c}| \quad \leq \quad 1 - \vec{b} \cdot \vec{c} \,. \tag{480}$$

This relation can easily be violated, assume e.g. $\vec{a}$, $\vec{b}$ and $\vec{c}$ lie in a plane, $\vec{a}$ and $\vec{b}$ are perpendicular and $\vec{c}$ lies in between them (with an angle of 45°). Then we get

$$|0 - 1/\sqrt{2}| = 0.707 \quad \leq \quad 1 - 1/\sqrt{2} = 0.29 \,, \tag{481}$$

which is obviously not correct.

Combing this result - hidden variable are not compatible with quantum mechanics[8] - with the result from EPR have two possible resolutions:

1. Quantum mechanics is wrong.

2. Locality does not hold in general.

All experimental tests have shown that Quantum mechanics is correct and that Bell's inequality is violated. It seems that locality does not hold and that there is an instantaneous collapse of the wave function.

We are still left with lack of understanding of the collapse of the wave function. Scientist tried to establish the collapse of the wave-function experimentally; this comes under the name of **quantum Zeno effect**, but there are currently no convincing hints.

16.5   More fancy interpretations

Many world theories from Hugh Everett in 1957 [34]. Everett was a PhD student of John Archibald Wheeler. The idea was later on worked out by Bruce de Witt and more recently by David Deutsch and Wojciech H. Zurek. This theory tries to explain the collapse of the wave function.

Wikipedia states "Many-worlds implies that all possible alternative histories and futures are real, each representing an actual "world" (or "universe"). In lay terms, the hypothesis states there is a very large, perhaps infinite number of universes, and everything that could possibly have happened in our past, but did not, has occurred in the past of some other universe or universes. "

- *To repeat this lecture:* Chapter [17.1-4] of [1]

- *To prepare for next lecture:* All of [1]

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[8]One can, however, construct some fancy hidden variable models for which Bell's inequality is not applicable.

17 Revision Lecture

The course covered four topics

1. Scattering

2. Quantum statistical mechanics

3. Relativistic Quantum mechanics

4. Interpretation of Quantum mechanics

17.1 Scattering

17.2 Quantum statistical mechanics

17.3 Relativistic Quantum mechanics

17.4 Interpretation of Quantum mechanics

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