Mathematical Aspects of Quantum Theory and Quantization

Peter Bongaarts

Institute Lorentz for Theoretical Physics

University of Leiden

The Netherlands

p.j.m.bongaarts[at]xs4all.nl
bongaart[at]lorentz.leidenuniv.nl

Summer School in Mathematics School of Geometry

May 29 -June 9, 2012

University Kasdi Merbah,
Ouargla, Algeria

Revised version: January 1, 2015

Acknowledgements :

In preparing these notes the mathematical erudition of my friend Henk Pijls has been indispensable.

My wife Adrienne gave essential support during the school and was also very helpful in practical matters.

Amine Bahayou, the main organizer of the school, deserves much praise for his tireless efforts.

The interest shown by the students was a great stimulus.

Contents

Lecture 3

3. Quantum Theory - Quantum Statistical Mechanics

Lecture 4

4. Physical Theories as Algebraic Systems

Lecture 5

5. *Quantization*

Lecture 6

6. Quantum Theory and Relativity

Appendix : Minkowski diagrams

Mathematical Aspects of Quantum Theory and Quantization

1. Quantum Theory. General Principles

1.1. Introduction

Let me begin with a quote by Galileo Galilei who in 1623 expressed his idea about the role of mathematics in physics clearly and convincingly in his book "Il Saggiatore (The Assayer)":

La filosofia è scritta in questo grandissimo libro che continuamente ci sta aperto innanzi a gli occhi (io dico l'universo), ma non si può intendere se prima non s'impara a intender la lingua, e conoscer i caratteri, ne' quali scritto. Egli è scritto in lingua matematica, e i caratteri son triangoli, cerchi, ed altre figure geometriche, senza i quali mezi è impossibile a intenderne umanamente parola; senza questi è un aggirarsi vanamente per un oscuro laberinto.

In English translation :

Philosophy is written in this vast book, which continuously lies open before our eyes (I mean the universe). But it cannot be understood unless you have first learned to understand the language and recognise the characters in which it is written. It is written in the language of mathematics, and the characters are triangles, circles, and other geometrical figures. Without such means, it is impossible for us humans to understand a word of it, and to be without them is to wander around in vain through a dark labyrinth.

This was true in the time of Galileo, when mathematics indeed meant just circles and triangles, now basic secondary school material. It is even more true at present when the mathematical basis of physics uses much more advanced mathematics: Hilbert spaces, Lie groups, manifolds. (Note that by "philosophy" Galileo means "natural philosophy", i.e. physics and astronomy.)

Here is a more recent quote by Dirac:

"During a seminar in Moscow University in 1955, when Dirac was asked to summarize his philosophy of physics, he wrote at the blackboard in capital letters : "Physical laws should have mathematical beauty". This piece of blackboard is still on display."

Mathematics and physics used to be in an obvious way a single integrated subject. Think of Archimedes, Newton, Lagrange, Gauss, more recently Riemann, Cartan, Poincaré, Hilbert, von Neumann,

Weyl, van der Waerden, Birkhoff, and many others. Lorentz, the great Dutch physicist, was offered a chair in mathematics, simultaneosly with a chair in physics at an other Dutch university. He chose the latter and became in 1878 the first professor of theoretical physics in Europe.

All this is a thing of the past. For most present day mathematicians, especially for the younger generation, physics has become a *terra incognita*. This happened gradually in the fifties. It is not completely clear why. The Bourbaki program has had certainly great merits for the development of mathematics. It revolutionized its language, which, however, strongly contributed to this separation from physics. Note that most of the great stars of Bourbaki, Weil, Dieudonné, Cartan (Henri, not Elie), Grothendieck, had no interest in physics at all. The growing publication pressure in academia leading to much ultra-specialization and short-term work is maybe another reason. Among the older generation of mathematicians there are still a few mathematicians for who physics is an essential part of their scientific interest, think of Atiyah, Manin, Connes. My lectures here will try to give a local, modest, very modest, microscopic push in the other direction.

What topics will be discussed in these lectures? The general subject is quantum theory, as a physical theory, but with an emphasis on its mathematical structure. The mathematics for this is functional analysis, Hilbert space theory, and more particular the theory of linear operators. I explain what is needed for this briefly in these notes. Quantum theory is in a very deep and essential manner a probabilistic theory. For this we need some fairly elementary probability theory. Again, I shall explain some of this in these lectures.

Classical and quantum physics are very different, certainly at first sight. Nevertheless, they can be shown to have very similar mathematical structures, when formulated as what I shall call *algebraic dynamical systems*. This leads to the subject of quantization, procedures to construct quantum theories from given classical theories, Weyl quantization, strict and formal deformation quantization.

We shall restrict ourself mainly to nonrelativistic physics, but discuss in the last lecture the merging of quantum theory and the special theory of relativity, raising problems that remain partly unsolved.

1.2. Mathematics and physics. General remarks

It is worth pausing for a moment to look at the differences between physics and mathematics.

• *Rigour*: The basis of mathematical thinking is logic. A mathematical theory has to precisely defined, with rigorously proven theorems. This is an absolute requirement, the only one. Heuristics, intuition, elegance are important, but in the end not decisive. A physical theory has to meet *two* requirements. One is that the soundness of the mathematics in which it is formulated. The second is that is has to agree with experiments. If it cannot be checked experimentally, than it is not a physical theory; it is science fiction (e.g. string theory). If it can be checked but does not agree with experiments, then it is a false theory. The condition of mathematical rigour have sometimes (temporarily) to be relaxed. In particle physics, quantum field theory, for instance, quantum electrodynamics predicts experimental results with an unbelievable precision, but generations of physicists and mathematicians have over the last seventy years tried in vain to provide it with a proper mathematical basis, but nobody doubts that it is a good physical theory.

Mathematics is disciplined human imagination; physics is investigation of the real world.

• *Domain of validity*: A physical theory has a *domain of applicability*. Classical mechanics, for instance, is valid for situations in which there are no very high velocities involved – near the velocity of light. After that the theory of relativity takes over. It is also only valid for macroscopic phenomena; in the microworld quantum theory is needed. Etc..

• *Approximation*: Very few calculations, theoretical procedures, solutions of problems are exact. The famous 2-dimensional Ising model is a rare exception.

The general situation in physics is *approximation*. Results are often calculated by means of expansion in power series in orders of parameters which describe the strength of the interaction, as a deviation from a simple known situation. One usually does not bother too much about the convergence of such a series. Or by an ever finer discretization of a continuum model. Or by computer simulation.

• *Dimensions*: Mathematicians do not always realize that quantities in a formula in physics are in general not pure numbers, but have a *dimension* and therefore take different numerical values for different systems of units. One has basic units of length [L], mass [M], time [T], etc.. Other quantities have derived dimensions, like velocity with the dimension $[LT^{-1}]$, linear momentum with $[MLT^{-1}]$, energy with $[ML^2T^{-2}]$. Sometimes other basic units are added, for instance for electric charge or temperature.

By fixing the numerical values of certain fundamental physical constants one may reduce the number of basic units. For example, in particle physics one usually takes the velocity of light $c = 1$ and Planck's constant $\hbar = 1$, with the result that in this field energy can be taken as the sole basic unit: all quantities have the dimension of a positive of negative power of the energy.

Dimensions have something to do with *scaling*. A physicist will immediately see that certain formulas are incorrect, for instant formulas in which the argument of an exponential or logarithm is a physical quantity which is not dimensionless.

• *Heuristics*: This plays a certain role in mathematics. Think of Edward Witten who got a Fields medal in 1990 for a number of brilliant heuristic conjectures and arguments that lead to new areas of mathematics. This is however an exception. The role of heuristic methods is much more important in physics. Large parts of physics books and papers are written in heuristic language, familiar to physicists, but making them harder for readers from mathematics. Two examples. The Dirac δ-function and its derivatives, later made by Laurent Schwartz into a rigorous part of functional analysis, the theory of distributions. The so called 'anticommuting c-numbers'.

The use of heuristic language is a convenient tool in physics, but it is also dangerous, as it may hide real problems, as it does, for example, in quantum field theory.

Two ways of teaching a physics. In the first one follows its historic development, in the second one formulates a theory in terms of one or more mathematical postulates, 'axioms', from which the full theory can be derived. There is something to be said for both methods. Most physics text books follow – more or less – the historical approach, usually neglecting the mathematical background; the axiomatic method has advantages for mathematics students. I shall

at various places illustrate this by discussing quantum phenomena in both ways. In any case, a certain knowledge of the history of physics should be part of a scientific education.

1.3. Historical remarks

Physics as we know it, a successful *combination of mathematical and experimental science*, began in sixteenth and seventeenth century Europe, even though ancient and medieval civilizations, those of China, India, Greece and the Arab world for instance, were already in the possession of a considerable body of scientific knowledge: insights in certain areas of astronomy and of pure and applied mathematics on the one hand and empirical knowledge of physical phenomena on the other hand. Here, in the midst of North Africa, the contribution of Arabs scientists, such as al-Tusi, al-Kwarizmi, al-Haytham, and many others, deserves to be mentioned. They not only preserved classical knowledge but also greatly extended it, laying in this manner the basis for the subsequent scientific revolution that led to modern mathematics and physics. See Ref.[12].

The nucleus of the new physical science was mechanics, describing the action of forces, in particular forces on moving bodies. It was built on the principles laid down first by Galileo and then more systematically by Newton, and was developed further into a beautiful mathematical theory by – among others – Lagrange, Laplace, Hamilton and finally Poincaré. Electricity and magnetism, studied experimentally from the fifteenth century onward, and later more theoretically, as separate phenomena, were brought together into a single theoretical framework in the second half of the nineteenth century by Maxwell. The basic notions in his *general theory of electromagnetism* were electric and magnetic *fields*, propagating in space as radiation, with light waves as a special case. In addition to this there was thermodynamics and statistical mechanics, the first a phenomenological framework for describing experimentally observed properties of heat, temperature and energy, the second a way of explaining these 'macroscopic' phenomena by statistical arguments from the 'microscopic' picture of atoms and molecules that gradually became generally accepted.

At the end of the nineteenth century, the result of all this was *classical physics*, a description of the physical world, believed by many to

be essentially complete. It consisted of two main components, Newton's classical mechanics, for the description of *matter*, Maxwell's theory of electromagnetism, for *fields* and *radiation*, together with laws governing the interaction between matter and radiaton.

1.4. Problems of classical physics

At the beginning of the twentieth century a few small but persistent problems remained, cracks in the walls of the imposing building of classical physics. One of these was the problem posed by the frequency spectra of light emitted by atoms and molecules, measured systematically and with great precision during the last half of the nineteenth century. These spectra were *discrete* ; their frequencies followed simple empirical rules, for which no theoretical explanation could be given. There was no way in which the classical picture of atoms and radiation could account for this. A second problem was the *aether*, a special medium that was assumed to fill empty space. The existence of this aether was thought to be necessary for the propagation of light waves through vacuum, but was forced to have very contradictory properties. These problems could not be solved within classical physics; fundamentally new physical ideas were needed, which were found in two new theories which emerged in the first half of the twentieth century.

1.5. Two revolutions

The two new theories that solved the problems of classical physics and broke resolutely with classical notions were the *special theory of relativity* and *quantum mechanics*. They led eventually to a thorough revision of the foundations of physics, with new ideas, in relativity on space and time, and in quantum mechanics on causality and determinism. In this process classical mechanics and classical electromagnetism were relegated to the role of practically useful approximations to an underlying more general picture.

The aether problem was solved by theory of relativity, created in 1905 by Albert Einstein. Space and time were no longer separate entities; the became intimately related, forming together a 4-dimensional affine space, in which the distinction between space and time was indeed relative and depended on the motion of the observer. The aether was abolished. Einstein later developed the

general theory of relativity with gravity the basic force, acting in a curved 4-dimensional space-time *pseudo-Riemannian manifold*.

Quantum theory solved the problem of atomic spectra. Its history started in 1913 with Bohr's ad-hoc theoretical model of the hydrogen atom. Scattering experiments by Rutherford had shown that such an atom was a system consisting of a positively charged heavy nucleus in the centre, encircled by a light electron with a negative charge. This very small planetary system emitted electromagnetic radiation, in certain discrete frequencies which could not be explained by classical physics. Bohr postulated in 1912 a model in which the electron could only move in a certain system of discrete orbits, jumping once in a while from one orbit to the next, radiating energy in this process.

Bohr's model had an immediate success. It had no theoretical justification at all, but it predicted not only the fact of the discreteness of the hydrogen spectral lines but also their frequencies in a fairly precise manner. This was the beginning of quantum theory.

1.6. Quantum mechanics

Quantum theory as we know it now was born in a period of a few years, roughly between 1924 and 1927, invented by Werner Heisenberg and Erwin Schrödinger, with important contributions by Max Born, Wolgang Pauli, Paul Dirac and many others. Immediately after this the mathematical foundations were laid by John von Neumann and group theory was introduced in quantum theory by Hermann Weyl.

Initially it looked as if there were two different and competing kinds of quantum theory: Heisenberg's matrix mechanics and, somewhat later, Schrödinger's wave mechanics. It soon turned out that they were just different faces of the same underlying mathematical model, a model that we shall describe in an explicit manner further on.

It is useful to distinguish between *quantum theory* and *quantum mechanics*. With quantum theory I mean the general theory. The special case of quantum mechanics describes mechanical systems with a finite number of degrees of freedom, i.e. a system of N (in general) interacting particles. Such a system has $6N$ degrees of freedom, $3N$ positions and $3N$ momenta. In most of my lectures, and certainly in

this lecture I shall restrict myself to nonrelativistic point particles, and at places even to a system of a single particle. Systems that do not belong to quantum mechanics proper are, for examples, spin systems, very important models for the description of solid matter in solid state physics, and systems with an infinite number of degrees of freedom such as quantum field theories in elementary particle physics. This will be discussed in my last lecture.

1.7. Axioms for quantum theory. The simplest situation

The basic properties of quantum theory can be expressed by a set of mathematical statements, 'axioms', together with their consequences. This system is essentially due to John von Neumann. The mathematics he used for it, most of it invented by him for this purpose, is functional analysis, in particular the theory of operators in Hilbert space. Here is the simplest version, to be called 'Version 1'.

Axiom I. ***The state of a physical system is described by a unit vector*** ψ ***in a Hilbert space*** $\mathcal{H}$***.***

Remark: Multiplication of a unit vector by a phase factor gives the same state. It means that, strictly speaking, the state space is not the Hilbert space $\mathcal{H}$ but the associated projective Hilbert space $P(\mathcal{H})$. We shall not bother about this.

Remark: A Hilbert space is a complex inner product space; the infinite dimensional version that quantum theory requires has additional topological properties necessary for discussing limits, in particular for taking the sum of infinite series. A vector ψ in $\mathcal{H}$ has a *norm* defined as $||\psi|| = \sqrt{(\psi, \psi)}$. Convergence of a sequence of vectors $\{\psi_n\}_{n\in N}$ to a limit ψ means $\lim_{n\to\infty} ||\psi - \psi_n|| = 0$. A Hilbert space is *complete*, i.e. every Cauchy sequence is convergent.

Axiom II. ***Observables are represented by selfadjoint operators*** A ***in*** $\mathcal{H}$*.*

Remark: A selfadjoint operator in a Hilbert space is the infinite dimensional generalization of a hermitian operator or matrix in ordinary linear algebra. However, due to the infinite dimension, operators in Hilbert space have much more subtle properties. They are often not defined on all of $\mathcal{H}$, but only on a dense linear subspace of $\mathcal{H}$, their *domain*. Such operators are called *unbounded*, for a reason that will be explained further on. A simple algebraic manipulation

as multiplication of two unbounded operators A and B is a non-trivial procedure, because the domains of A and B have to match. Unfortunately, many or most of the operators in quantum theory are of this type.

An operator A in $\mathcal{H}$ is called *hermitian*, or *symmetric*, if

$$(\psi_1, A\psi_2) = (A\psi_1, \psi_2), \quad \forall \psi_1, \psi_2,$$

the standard definition from linear algebra, which for unbounded operators has to be supplemented by the condition "for all ψ_1 and ψ_2 in the domain of definition of A". Hermiticity of operators is not good enough for the case of the unbounded operators in quantum theory; we need the property of *selfadjointness*, which is stronger. Its definition is rather technical. We refrain from giving it here.

1.8. An explicit example

Before going on to the next axioms it is good to understand these two first by looking at a simple explicit example. The obvious one, both from a historical as well from a pedagogical point of view, is the Schrödinger theory for the description of a single point particle in a given external potential, such as the Coulomb potential in the model of the hydrogen atom.

Ad Axiom I: The Hilbert space of state vectors $\mathcal{H}$ is the space of complex-valued square integrable functions $L^2(R^3, d\vec{x})$ with $d\vec{x} = dx_1 dx_2 dx_3$. The elements of this space are the wave functions $\psi(\vec{x})$, with $\vec{x} = (x_1, x_2, x_3)$. The inner product of two wave functions ψ_1 and ψ_2 is

$$\int_{-\infty}^{+\infty} \overline{\psi_1}(\vec{x})\psi_2(\vec{x})\, d\vec{x}.$$

Note that this is the physics convention: the inner product is conjugate linear in the first variable.

Note that the wave function for the description of a state of N particles is a function of $3N$ variables, e.g. for a two particle system one has $\psi(\vec{x}^{(1)}, \vec{x}^{(2)})$.

Ad Axiom II: The basic observables in the classical description a single point particle are the variables for position x_1, x_2, x_3 and momentum p_1, p_2, p_3, and from these all others are constructed, in par-

ticular the most important one, the total energy

$$H = \frac{\mathbf{p^2}}{2m} + V(x_1, x_2, x_3),$$

with $\mathbf{p} = \sum_{\mathbf{j=1}}^{\mathbf{3}} \mathbf{p_j^2}$ and m the mass of the particle. In quantum mechanics the corresponding operators are those for position, multiplication operators Q_j, acting as

$$(Q_j\psi)x_1, x_2, x_3) = x_j\psi(x_1, x_2, x_3),$$

for $j = 1, 2, 3$, and for momentum differentiation operators P_j, defined as

$$(P_j\psi)(x_1, x_2, x_3) = \frac{\hbar}{i}\frac{\partial}{\partial x_j}\psi(x_1, x_2, x_3),$$

for $j = 1, 2, 3$. Note the appearance of $\hbar$ in this formula. This is Planck's constant, a constant of nature, typical for quantum theory, and appearing in all quantum theoretical formulas. The energy as an observable is represented, not surprisingly, by the operator

$$H = \frac{\mathbf{P^2}}{2m} + V,$$

with V the multiplication operator

$$(V\psi)(x_1, x_2, x_3) = V(x_1, x_2, x_3)\psi(x_1, x_2, x_3).$$

It is not hard to verify that all these operators are unbounded. For ψ a square integrable function $Q_j\psi$ need not to be square integrable; this requirement determines the domain of definition of Q_j. Similarly, the operator P_j is defined only on differentiable functions; moreover the resulting function$P_j\psi$ should be square integrable. It is also not difficult to check that the Q_j and P_j are hermitic. That they are also selfadjoint is a nontrivial property that we shall not prove here.

Note that this simple prescription of obtaining a function of certain operators by following the classical expression does not work in general. It is alright with the operator H but problematic already with a simple expression like P_jQ_j. This is because we have for the classical variables $p_jq_j = q_jp_j$; for the quantum variables $P_jQ_j \neq Q_jP_j$, as will be clear from what follows.

The operators P_j and Q_j, the 'canonical operators' as they are called, have interesting relations, not difficult to derive, the *canonical commutation relations*,

$$[P_j, P_k] = [Q_j, Q_k] = 0, \qquad [P_j, Q_k] = \frac{\hbar}{i}\,\delta_{jk}, \qquad j,k = 1,2,3.$$

These formulas are emblematic for quantum mechanics. There is an important uniqueness theorem, the Stone - von Neumann theorem, which, among other things, states that for a given n all irreducible systems of such operators $\{P_j\}_{j=1,\ldots,n}$ and $\{Q_k\}_{k=1,\ldots,n}$ are unitarily equivalent. (A system of operators $\{A_\rho\}_\rho$ in a Hilbert space $\mathcal{H}$ is called irreducible if and only if an operator that commutes with all the members of this system is necessarily a scalar multiple of the unit operator. Two systems $\{A_{\rho_1}\}_{\rho_1}$ and $\{A_{\rho_2}\}_{\rho_2}$ in $\mathcal{H}_1$ and $\mathcal{H}_2$ are called unitarily equivalent if and only if there exist a unitary map $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $A_{\rho_2} = UA_{\rho_1}U^{-1}$, for all ρ.)

1.9. Axioms for quantum theory. Continued

The third axiom, part A, describes the *physical interpretation* of the combination of axioms I and II, for the case of a single observable.

Axiom III$_0$. **The probability of measuring the value α for the observable A in a state ψ is given by a distribution function $F(\alpha) = (\psi, E_\alpha\psi)$, with E_α a spectral projection of the operator A.**

Remark: This axiom is the central statement of the quantum theoretical formalism. For this we use what is the main theorem in the mathematical formulation of quantum theory, the *spectral theorem for selfadjoint operators in Hilbert space*. It is a non-trivial generalization of the well-known fact from elementary finite dimensional linear algebra that a hermitian matrix has an orthonormal basis of eigenvectors, for real eigenvalues.

Here is a reminder of this finite dimensional case. Let $\{A_{jk}\}_{jk}$ be a $n \times n$ hermitian matrix, or equivalently, a hermitian operator in a complex n-dimensional inner product space. It is an elementary theorem in linear algebra that A has an orthogonal basis of eigenvectors ϕ_j with real eigenvalues α_l, i.e. with $A\phi_j = \alpha_j\phi_j$, which allows us to write A as

$$A = \sum_{j=1}^{n} \alpha_j E_j,$$

in which the E_j are the orthogonal projections on $\{\phi_j\}_j$. We may call the numbers $\{\alpha_j\}_j$ the *spectrum* of A, and the projections $\{E_j\}_j$ *spectral projections*. This is the spectral theorem for a hermitian matrix or operator in an n-dimensional complex inner product space.

If the Hilbert space is infinite dimensional – I shall reserve the name Hilbert space for this situation, even though this is not quite the standard usage – the situation becomes more complicated. In the first place we have to replace the notion of hermitian operator by that of *selfadjoint*. There is still the possibility that a selfadjoint operator has only a discrete spectrum, i.e. eigenvalues in proper sense – we shall meet an example further on. In that case we still have the above sum formula, now with the summation running from 1 to ∞. In the general case there will be either discrete or continuous spectrum, or a combination of both.

To understand this we go back to our explicit example. But first a few remarks on probability theory.

Probability theory: Probabilistic ideas are essential in quantum theory. Most of what we need in this respect is fairly elementary. Here is a reminder of some basic facts:

1. Discrete probabilities: there is a discrete set of possibilities, finite or countably infinite, the *sample space*. Probabilities on this means a *sequence* $(\rho_1, \rho_2, \ldots)$ of nonnegative numbers, with $\sum_j \rho_j = 1$. Such a number ρ_j is the probability of finding the system in the j^{th} possibility. The average value (mean value) of what is called a discrete stochastic variable, a sequence $(g_1, g_2, \ldots)$, is $< g >= \sum_j g_j \rho_j$. Its n^{th} moment is $< g^n >= \sum_j g_j^n \rho_j$.

2. Continuous probabilities: The sample space is a nondiscrete set, for instance an interval $[a, b]$, the full real line R^1, or a suitable part of R^n, etc.. Probability on such a space is a *probability density*, a nonnegative function $\rho(x)$ with $\int \rho(x)dx = 1$. The probability of finding the system in the interval $[x_1, x_2]$ is $\int_{x_1}^{x_2} \rho(x)dx$. The average value (mean value) of a stochastic variable g is $< g >= \int g(x)\rho(x)dx$; its n^{th} moment is $< g^n >= \int g(x)^n \rho(x)dx$.

Strictly speaking, there are three kinds of probabilities: discrete, then continuous, with a probability density, which is called absolutely continuous, and finally a third possibility, called singular continuous. We shall not bother about this last possibility.

There is a convenient way of formulating the two (in fact three) sorts of probabilities in sequence sample spaces and subsets of R^1 in a single manner, by means of the notion of a *distribution function*. For the discrete case we define

$$F(x) = \sum_{j=1}^{j \leq x} \rho_j,$$

and for the continuous case

$$F(x) = \int_{-\infty}^{x} \rho(x) dx.$$

In both cases F is a monotone nondecreasing function, continuous from the left, with

$$\lim_{x \to -\infty} F(x) = 0, \qquad \lim_{x \to +\infty} F(x) = 1.$$

For the discrete case F is a step function. Averages are calculated with a *Lebesgue-Stieltjes integral*; for a stochastic variable g – in the discrete case written as a step function – this means

$$< g >= \int_{-\infty}^{+\infty} g(x)\, dF(x),$$

with the n^{th} moments

$$< g^n >= \int_{-\infty}^{+\infty} g(x)^n\, dF(x).$$

It should be noted that probability theory, certainly as far as its basic mathematical concepts are concerned, is a part of the theory of measure and integration. A probability space is, in technical terms, nothing but a measurable space with a measure of total mass equal to 1; with stochastic variables measurable functions on this space.

With these probabilistic ideas we can develop further the meaning of Axiom III_0., in particular the meaning of the general spectral theorem, in the case where we no longer have proper eigenvalues and eigenvectors.The general spectral theorem for a selfadjoint operator A in an infinite dimensional Hilbert space is

$$A = \int_{-\infty}^{+\infty} \alpha\, dE_\alpha\,,$$

a vector-valued Stieltjes integral, which we may see, if we wish, as the representation of a collection of numerical Stieltjes integrals

$$(\psi, A\psi) = \int_{-\infty}^{+\infty} \alpha \, d(\psi, E_\alpha \psi),$$

for all unit vectors ψ in the domain of definition of the operator A.

1.10. Back to our simple model

To understand how the probabilistic ideas just presented are helpful to understand the eigenfunction / eigenvector problem of general selfadjoint operators, we return to our simple explicit example. We make it even simpler, just for the case of notation, and restrict it to a particle in a potential in 1-dimensional space. This means that the Hilbert space $\mathcal{H}$ is $L^2(R^1, dx)$, with wave functions $\psi(x)$, a single position operator Q and a single momentum operator P, with the canonical commutation relation $[P, Q] = -i1_{\mathcal{H}}$. The eigenvalue / eigenfunction equation for the operator P is

$$(P\psi)(x) = \lambda\psi(x)$$

For every real value p of λ, it has as solution the function

$$\varphi_p(x) = C \, e^{\frac{i}{\hbar}px},$$

with C an arbitrary nonzero constant. However, these functions are not square integrable, they are *not* vectors in $\mathcal{H}$. (They represent plane waves with wave lenght $2\pi\hbar/p$. As such they are often used heuristically in physics text books, even they though they are inadmissible as quantum state vectors). In the strict sense P has neither eigenvalues nor eigenfunctions. Nevertheless, one says that P has a continuous spectrum, the full real line. There are no eigenvectors, so no projection operators to use in a formulation of the spectral theorem, as we did for the finite dimensional case. For this there exists a more subtle sort of what are called *spectral projections*. The simplest way to introduce these is by looking at the operator Q. Its eigenvalue / eigenfunction problem is

$$(Q\varphi)(x) = \lambda\varphi(x).$$

Suppose there is a solution $\phi(x)$ for the eigenvalue $\lambda = \lambda_0$. This means $(x - \lambda_0)\phi(x) = 0$, implying $\varphi(x) = 0$, for all $x \neq 0$. In an L^2

sense it is identicaly zero, so again not a proper quantum mechanical wave function. However, also in this case the operator has as continuous spectrum the full real line. There are again spectral projections, taking the place of the projections on the eigenvectors in the discrete case. For the operator Q they are easy to demonstrate. First however a note on projection operators.

A reminder on projection operators: Projection operators in Hilbert space can be defined in two equivalent ways :

1. *Algebraic*: A linear operator E in a Hilbert space $\mathcal{H}$ is a projection (short for projection operator) if and only if

$$E^2 = E, \qquad E^* = E,$$

i.e. if it is idempotent and selfadjoint.

2 *Geometric*: A projection operator E in $\mathcal{H}$ maps all vectors orthogonally on a (closed) linear subspace $\mathcal{M}$ of $\mathcal{H}$.

Properties:
1. A projection operator is a bounded operator.
2. Two projections E_1 and E_2 have the relation $E_1E_2 = E_2E_1 = E_1$, if and only if one has for the corresponding subspaces $\mathcal{M}_1 \subset \mathcal{M}_2$. This implies that there is a *partial order* $\prec$ in the set $\mathcal{E}(\mathcal{H})$ of all projections in $\mathcal{H}$.
3. A projection E has a complement, denoted as $E^\perp$ and defined as $E^\perp = 1 - E$. If E projects on $\mathcal{M}$, then $E^\perp$ projects on its orthogonal complement $\mathcal{M}^\perp$.
4. One has as trivial projection the operators 0 and 1.

Back to our 1-dimensional quantum mechanical model. Define for every real number x_0 the operator E_{x_0} in $\mathcal{H} = L^2(R^1, dx)$, according to

$$(E_{x_0}\psi)(x) = \psi(x), \text{ for } x \leq x_0, \text{ and } = 0, \text{ for } x > x_0$$

This is a projection on the subspace of $\mathcal{H}$ consisting of all functions that vanish for $x > x_0$.

The system $\{E_x\}_{x \in R^1}$ has the following important and characteristic properties, not difficult to verify,

1. $E_{x_1}E_{x_2} = E_{x_2}E_{x_1}, \quad \forall x_1, x_2 \in R^1$ (commutativity),
2. $x_1 \leq x_2 \rightarrow E_{x_1} \prec E_{x_2}$ (monotone nondecreasing),
3. $\lim_{x \uparrow x_0} E_x = E_{x_0}$ (continuity from the left),

4. $\lim_{x\to-\infty} E_x = 0$, $\lim_{x\to+\infty} E_x = 1$.

The system $\{E_x\}_{x\in R^1}$ is by definition the *spectral resolution* of the operator Q.

Note that limits in point 3 are limits for operator-valued functions. There are various notions of such limits. We shall say something about this later on. In any case this set of operator properties gives rise to an equivalent system of complex number-valued set of properties:

Let ψ be an arbitrary unit vector in $\mathcal{H}$. Then the expression $(\psi, E_x\psi)$ has the following properties, implied immediately by the properties 1,2 and 3 of the system $\{E_x\}_{x\in R^1}$,

1. $x_1 \le x_2 \;\to\; (\psi, E_{x_1}\psi) \le (\psi, E_{x_2}\psi)$.

2. $\lim_{x\to-\infty}(\psi, E_x\psi) = 0$, $\lim_{x\to-+\infty}(\psi, E_x\psi) = 1$, for all unit vectors in $\mathcal{H}$.

If we denote $F_\psi(x) = (\psi, E_x\psi)$, then the properties 1 and 2 show that $F_\psi(x)$ is a distribution function in the sense of probability theory, a notion that we discussed earlier. Distribution functions are the vehicles to express the physical meaning of the spectral theorem for selfadjoint operators. For the position operator Q this theorem is indeed

$$Q = \int_{-\infty}^{+\infty} x\, dE_x,$$

as an operator-valued Stieltjes integral, or as

$$\int_{-\infty}^{+\infty} x\, d(\psi, E_x\psi) = \int_{-\infty}^{+\infty} x\, dF_\psi(x),$$

for all unit vectors ψ in $\mathcal{H}$, as an equivalent system of numerical Stieltjes integrals. It is clear that all the distribution functions $F_\psi(x)$ are not only real monotone nondecreasing functions, but also continuous. This signifies the fact that the spectrum of the operator Q is continuous and consists of all real numbers.

Exhibiting the spectral resolutions and the spectral theorem for the momentum operator P is a bit more involved. For this we need the Fourier transforms of the wave functions,

$$(\mathcal{F}\psi)(p) := \widehat{\psi}(p) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x) e^{-\frac{i}{\hbar}px}\, dx,$$

with its inverse

$$(\mathcal{F}^{(-1)}\widehat{\psi})(x) := \psi(x) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \widehat{\psi}(p) e^{+\frac{i}{\hbar}px}\, dp,$$

The Fourier transformation is a operator which maps the function space $\mathcal{H} = L^2(R^1, dx)$ onto the function space $\widehat{\mathcal{H}} = L^2(R^1, dp)$. The Plancherel theorem, connected with this,

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{+\infty} |\hat{\psi}(p)|^2\, dp$$

states that $||\mathcal{F}\psi||^2 = ||\psi||^2$, which expresses the unitarity of the transformation $\mathcal{F}$. In this, what is called *momentum representation*, P acts also as a multiplication operator

$$(P\widehat{\psi})(p) = p\widehat{\psi})(p).$$

The further development is very similar to what is done in the case of the position operator Q, i.e. definition of a system of projection operators $\{E_p\}_p$ in the Hilbert space of functions $\widehat{\mathcal{H}}$, definition of the distribution functions $F_{\widehat{\psi}}$, for every $\widehat{\psi}$ in $\widehat{\mathcal{H}}$, and finally the statement of the spectral theorem as

$$P = \int_{-\infty}^{+\infty} p\, dE_p.$$

Also in this case the spectrum consists of all real numbers.

The operator Q in $\mathcal{H}$ is a multiplication operator, in analogy with finite dimensional linear algebra it may be said to be represented 'diagonally'. This is not so for the operator P in $\mathcal{H}$, but P is made 'diagonal' by the unitary transformation $\mathcal{F}$ from $\mathcal{H}$ onto $\widehat{\mathcal{H}}$. In finite dimensional linear algebra bringing a hermitian matrix in diagonal form by a unitary transformation is the essence of solving the eigenvalue / eigenvector problem. What we have done here is the infinite dimensional generalization of this.

Knowing the mathematics, the eigenvalue / eigenvector problem for Q and P – or rather the problem of finding the appropriate spectral resolutions – is easy, as we have seen. For the Hamiltonian operator, the energy operator, although a simple expression in position and momentum, this is a separate problem, much more difficult, except in the case where the particle is free, i.e. when the potential V is

identically zero, not an exciting case, of course, when the Hamiltonian is just a function of the momentum alone, n.l. $H_0 = \vec{p}^2/2m$. Depending on the potential V the spectrum may be completely discrete (the harmonic oscillator), completely continuous (the free particle) or mixed (the hydrogen atom). This is due to the fact that this expression contains noncommuting operators, the occurrence of which is a central feature of quantum theory. Solving the eigenvalue / eigenvector problem for the energy is the most important physical problem in almost all concrete quantum mechanical models. Exact solutions are rare exceptions; laborious approximate solutions in terms of power series expansions are the rule.

1.11. The general Axiom III

Axiom III_0 described the interpretation of Axioms I and II for a single observable. We now state Axiom III for the general case of a system of what we call *'commensurable' observables*, i.e. a system of observables represented by *commuting selfadjoint operators*. This adjective is crucial in what follows. Note that for two unbounded selfadjoint operators A and B, a common situation in quantum theory, their domains of definition may not match, so the products AB and BA may not be defined properly. To avoid this problem selfadjoint operators are said to commute if and only if all their spectral projection operators – which are bounded – commute.

Axiom III (general): **A unit vector ψ, representing a state of a quantum system, together with n commuting selfadjoint operators $A_1, \ldots, A_n$, representing observable quantities $a_1, \ldots, a_n$, determines a system of stochastic variables. The simultaneous distribution function for these variables is given by**

$$F_\psi(\alpha_1, \ldots, \alpha_n) = (\psi, E_{\alpha_1 \ldots \alpha_n}\psi),$$

with the projection operators $E_{\alpha_1 \ldots \alpha_n}$ forming the n-parameter spectral resolution associated with the system $A_1, \ldots, A_n$.

This axiom completes the physical interpretation of Axiom I and Axiom II.

Ad Axiom III : For this axiom we need a further remark on probability theory.

In standard probability any set of stochastic variables $(g_1, \ldots, g_n)$ has a joint (sometimes called simultaneous or cumulative) distribution function $F(x_1, \ldots, x_n)$, defined similarly to the case of a single variable that we discussed earlier, both for the discrete as well as the continuous case. For a pair of variables one has a correlation function, and conditional probabilities, expressing the probability for a certain outcome for a_2, given the result for a_1. By integrating out $n-1$ variables in an n-dimensional distribution function, one obtains a 1-dimensional distribution function in the remaining variable. All this is of no great interest in the present context.

The spectral theorem for a set of commuting selfadjoint operators $(A_1, \ldots, A_n)$ states that there exists a joint spectral family, a system of projection operators $E_{\alpha_1,\ldots,\alpha_n}$ such that every A_j can be written as

$$A_j = \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} \alpha_j \, dE_{\alpha_1,\ldots,\alpha_n}.$$

The set of projections has the properties

1. $E_{\alpha_1,\ldots,\alpha_n} E_{\alpha'_1,\ldots,\alpha'_n} = E_{\alpha'_1,\ldots,\alpha'_n} E_{\alpha_1,\ldots,\alpha_n}$,
   for all $\alpha_1, \ldots, \alpha_n$ and $\alpha'_1, \ldots, \alpha'_n$, (commutatitivity),

2. $\alpha_j \leq \alpha'_j, \quad \alpha_k = \alpha'_k, \quad k \neq j \quad \rightarrow \quad E_{\alpha_1,\ldots,\alpha_j\ldots,\alpha_n} \prec E_{\alpha_1,\ldots,\alpha'_j,\ldots,\alpha_n}$,
(monotone nondecreasing,

3. $\lim_{\alpha_j \to -\infty} E_{\alpha_1,\ldots,\alpha_j\ldots,\alpha_n} = 0, \quad \lim_{\alpha_j \to +\infty} E_{\alpha_1,\ldots,\alpha_j\ldots,\alpha_n} = 1$
   for $j = 1, \ldots, n$.

These projections give simultaneous distribution functions, for each ψ in $\mathcal{H}$,

$$F_\psi(\alpha_1, \ldots, \alpha_n) = (\psi, E_{\alpha_1,\ldots,\alpha_n}\psi).$$

For the three position operators Q_1, Q_2 and Q_3 in our simple 3-dimensional model this implies that the probability of finding the particle in a cube with sides $[x_1^a, x_1^b]$, $[x_2^a, x_2^b]$and $[x_3^a, x_3^b]$ is given by

$$\int_{x_1^a}^{x_1^b} \int_{x_2^a}^{x_2^b} \int_{x_3^a}^{x_3^b} dF_\psi(x_1, x_2, x_3) =$$

$$= \int_{x_1^a}^{x_1^b} \int_{x_2^a}^{x_2^b} \int_{x_3^a}^{x_3^b} ||\psi(x_1, x_2, x_3)||^2 \, dx_1 dx_2 dx_3,$$

because the operators Q_j have continuous spectrum and the probability can therefore be given by the probability density

$$\rho(x_1, x_2, x_3) = ||\psi(x_1, x_2, x_3)||^2.$$

Note that this means that we can determine the position of a particle with arbitrary precision, by taking the sides of the cube arbitrary small. But these sides cannot be zero; there is no state for a particle at an exact position (x_1^0, x_2^0, x_3^0), even though improper state vectors, pretending to describe such a situation, are widely used in a heuristic manner in physics books. Examples are 'states' described by Dirac δ-functions for positions, and plane wave functions for momentum, mentioned already. But in a mathematically rigorous formulations these improper states have no place.

1.12. Noncommensurable observables

For the interpretation of Axioms I and II, for explaining what it means to measure an observable or a set of of observables, we needed only classical probability theory. This is because we only admitted systems of *commensurable observables*, observables represented by *commuting* selfadjoint operators. As long as one considers these, one may say quantum mechanics is a part of standard classical probability theory.

This changes drastically if one takes into account systems of *incommensurable observables*. This leads to the heart of what makes quantum theory nonclassical.

Important pairs of incommensurable observables are the components of position and momentum in the same direction, as is clear from the canonical commutation rules for the operators P_j, Q_k that we discussed. Also important is the triple of components of angular momentum. The classical angular momentum of a particle with respect to the origin is, in vector notation, $\vec{l} = \vec{x} \times \vec{p}$, or in components

$$l_{x_1} = x_2 p_3 - x_3 p_2,$$

$$l_{x_2} = x_3 p_1 - x_1 p_3,$$

$$l_{x_3} = x_1 p_2 - x_2 p_1,$$

The associated selfadjoint operators $\vec{L} = \vec{Q} \times \vec{P}$, in components (L_1, L_2, L_3), have the commutation relations

$$[L_1, L_2] = i\hbar L_3,$$

$$[L_2, L_3] = i\hbar L_1,$$
$$[L_3, L_1] = i\hbar L_2,$$

which means that in quantum mechanics the observables of angular momentum in different directions are incommensurable. Note that one can consider the operator

$$L^2 = (L_1)^2 + (L_2)^2 + (L_3)^2,$$

which commutes with all three components L_j, as one checks easily, so it is convenient to use a pair (L^2, L_j), usually (L^2, L_3) as of commensurable variables, for which one can solve the simultaneous eigenvalue / eigenvector problem.

The main quantum principle is that there is no simultaneous probability distribution for a pair of incommensurable observables.

Each observable can be measured separately, with a probability distribution of its own. For a given state they are not independent; instead of a joint distribution there are restrictions on the results of the separate measurements. We shall derive a general inequality which gives such a restriction and after that apply the result two incommensurable quantities in our simple explicit example.

Suppose we have a quantum theory with as state space a Hilbert space $\mathcal{H}$. Let A and B be two noncommuting selfadjoint operators in $\mathcal{H}$, corresponding with observables a and b. Choosing a vector ψ in $\mathcal{H}$ determines according to Axiom III_0, two stochastic variables a_ψ and b_ψ, in fact both classical variables, with distribution functions $F_{a_\psi}(\alpha)$ and $F_{b_\psi}(\beta)$, and with expected values $< a_\psi >$ and $< b_\psi >$, defined separately by the spectral theorem for A and B. They also have standard deviations, a notion defined earlier,

$$\Delta a_\psi = \sqrt{< (a_\psi - < a_\psi >)^2 >}, \qquad \Delta b_\psi = \sqrt{< (b_\psi - < b_\psi >)^2 >}.$$

In classical probability theory a pair of stochastic variables a and b have not only separate distribution functions $F_1(\alpha)$ and $F_2(\beta)$ but also a joint distribution function $F_{12}(\alpha, \beta)$, from which one can in fact derive F_1 and F_2 by integrating over β and α. The two variables can be measured *simultaneously*, and with arbitrary precision. This was still the case for a pair of commensurable quantum observables, as we have seen.

For incommensurable quantum variables, i.e. represented by non-commuting operators A and B, this is no longer true. Both observables can still be measured separately for a given state, each on its own with arbitrary precision, but it is not possible to do this simultaneously. In fact there is a *restriction* depending on the 'amount of noncommutativity' of A and B.

There is a very useful tool in Hilbert space theory: the *Schwarz inequality*.

$$|(\psi_1, \psi_2)| \leq ||\psi_1||||\psi_2||.$$

for all vectors ψ_1 and ψ_2 in $\mathcal{H}$, with the addition that there is equality if and only if ψ_1 is a scalar multiple of ψ_2. The proof of this is a good, not too difficult exercise in Hilbert space theory. However, we refrain from giving it here. The Schwarz inequality is sometimes called the *Cauchy-Schwarz inequality*.

Using the Schwarz inequality one can prove the basic 'quantum inequality'

$$\Delta a_\psi \, \Delta b_\psi \geq \frac{1}{2}(\psi, [A, B]\psi).$$

In this formula we have the *standard deviations* Δ, or *spreads*,

$$\Delta a_\psi = \sqrt{<(a_\psi - < a_\psi >)^2>},$$

$$\Delta b_\psi = \sqrt{<(b_\psi - < b_\psi >)^2>}.$$

This inequality is the *general uncertainty relation* for the standard deviations of two observables a and b in the state ψ. It is a restriction on the possible outcomes of a simultaneous measurement of a and b. For commensurable a and b, i.e. for commuting A and B, there is, evidently, no restriction.

We apply this to the 1-dimensional quantum mechanical model, where we have a pair of incommensurable observables, position and momentum. The corresponding operators have the commutation relation

$$[P, Q] = -i\hbar 1_{\mathcal{H}},$$

with as a consequence the *Heisenberg uncertainty relation* for position and momentum

$$\Delta p \, \Delta x \geq \frac{\hbar}{2}.$$

Note that we write here Δx and Δp instead of Δx_ψ and Δp_ψ because the right-hand side no longer depends on the state vector ψ, as one sees immediately. The Heisenberg uncertainty relation is an iconic formula, probably the best known of all formulas of quantum mechanics, one of the centre pieces of elementary quantum mechanics, illustrating the fundamental incommensurability of position and momentum. For the 3-dimensional case one has

$$\Delta p_j \, \Delta x_j \, \geq \, \frac{\hbar}{2} \qquad j = 1, 2, 3.$$

1.13. Time evolution

After the first three axioms the next two are less surprising, because the natural automorphisms of a Hilbert space, as a mathematical structure, are unitary operators

A mathematical reminder: A *unitary operator* in a Hilbert space $\mathcal{H}$ is an invertible map from $\mathcal{H}$ onto itself with the property

$$U^* U = U U^*,$$

implying $U^* = U^{-1}$. An equivalent definition is

$$(U\psi_1, U\psi_2) = (\psi_1, \psi_2), \quad \forall \psi_1, \psi_2 \in \mathcal{H},$$

or

$$||U\psi|| = ||\psi||, \quad \forall \psi \in \mathcal{H}.$$

A 1-parameter group of unitary operators is a system $\{U(t)\}_{t \in R^1}$ with the properties

1. $U(0) = 1$,

2. $U(t_1)U(t_2) = U(t_1 + t_2), \quad \forall t_1, t_2 \in R^1$,

implying $U(-t) = U(t)^{-1}$.

Limits for operators: Vectors ψ have a norm $||\psi|| = (\psi, \psi)^{1/2}$. Bounded operators also have a norm

$$||A|| =: \sup_{||\psi||=1} ||A\psi||.$$

A sequence of bounded operators $\{A_n\}_{n=1,2\ldots}$ *converges in norm* to an operator A if and only if $\lim_{n \to +\infty} ||A - A_n|| = 0$. The topology associated with this convergence is too strong for most applications.

There is a weaker topology, strangely enough called the strong operator topology. A sequence of bounded operators $\{A_n\}_{n=1,2...}$ *converges in strongly* if and only if $\lim_{n\to+\infty} ||A\psi - A_n\psi|| = 0$, for all ψ in $\mathcal{H}$. There a many other topologies / notions of convergence in Hilbert space theory. Fortunately, we do not need them.

Axiom IV: **Time evolution in quantum theory is described by a strongly continuous 1-parameter group of unitary operators $\{U(t)\}_{t\in R^1}$, acting in the Hilbert space of states $\mathcal{H}$.**

The mathematical basis for this axiom, *Stone's theorem*, is the second most important theorem for quantum theory. It states that a strongly continuous 1-parameter group $\{U(t)\}_{t\in R^1}$ can be written as an exponential $U(t) = e^{iAt}$, with the generator A a selfadjoint operator.

For the time evolution in quantum theory this generator is the Hamiltonian operator H, in most cases also the energy as an observable. So we have $U(t) = e^{\frac{i}{\hbar}tH}$, with $\hbar$, Planck's constant included.

An observable is a *constant of the motion* or *conserved quantity* if and only if the corresponding selfadjoint operator commutes with H, or equivalently, with the $U(t)$, for all times t. A state ψ is called a *stationary state* if the probabilities of measurements of *all observables* are constant in time.

With this the time evolution for a state vector ψ is written as

$$\psi(t) = e^{-\frac{i}{\hbar}tH}\psi(0).$$

The $\psi)t)$ satisfy a vector-valued ordinary first order differential equation, the *'abstract' Schrödinger equation*

$$\frac{d}{dt}\psi(t) = -\frac{i}{\hbar}H\psi(t).$$

In our concrete model of a particle in 3-dimensional space we obtain the *'standard' Schrödinger equation*, as a partial differential equation of mixed order, appearing in all text books on quantum mechanics,

$$\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta\psi(\vec{x},t) + V(\vec{x})\,\psi(\vec{x},t)\right].$$

It sometimes more convenient to describe time evolution not in what is called the *Schrödinger picture*, but in the *Heisenberg picture*. This means that one keeps the state vectors constant in time, and puts the time dependence in the operators for the observables:

$$A_h(t) =: e^{\frac{i}{\hbar}tH} A_s e^{-\frac{i}{\hbar}tH}.$$

As all numerical results are calculated by using the inner product, this has no effect on the physical content.

1.14. Symmetry

Symmetry is a very important notion in physics. It simplifies the solution of concrete problems and is often a guide in finding new models for physical phenomena.

The symmetries of a mathematical object are its *automorphisms*, i.e. the invertible maps from the object onto itself, which leave its characteristic structure invariant. For a Hilbert space these are the unitary operators. A quantum theory, as a mathematical object a pair $(\mathcal{H}, \{U(t)\}_{t\in R})$, consisting of a Hilbert space of states $\mathcal{H}$ and a 1-parameter group $\{U(t)\}_{t\in R}$ of unitary time-evolution operators, has as its symmetry automorphisms the unitary operators in $\mathcal{H}$ that commute with all the unitary operators $U(t)$ of the time-evolution group, or equivalently with the selfadjoint generator H of this group. We state therefore as basic principle:

Axiom V: **Symmetries in quantum theory are described by unitary operators which commute with the 1-parameter group of time involution, or equivalently, with its generator, the Hamiltonian.**

Examples of elementary symmetries in quantum mechanics are *space reflection*, for example when the particle is moving in a potential V with $V(\vec{x}) = V(-\vec{x})$ or $V(|\vec{x}|)$, *space translation* for a system of two particles with $V(\vec{x}_1, \vec{x}_2) = V(\vec{x}_1 - \vec{x}_2)$, and *rotation in space* for a 3-dimensional particle moving in a rotation invariant potential.

Of particular importance are *groups of symmetries*.

Reminder: A *group* is a non-empty set $\mathcal{G}$ with the following properties:

1. There is a multiplication, i.e. a map $\mathcal{G} \times \mathcal{G} \to \mathcal{G}$, $(g_1, g_2) \mapsto g_1 g_2$, which is associative, which means that $(g_1 g_2)g_3 = g_1(g_2 g_3)$, for all g_1, g_2 and g_3 in $\mathcal{G}$.

2. $\mathcal{G}$ has a unit element e with $ge = eg = g$, for all g in $\mathcal{G}$.

3. Each g in $\mathcal{G}$ has an inverse, denoted as g^{-1}, which has the property $gg^{-1} = g^{-1}g = e$, for all g in $\mathcal{G}$.

A group may have the structure of a manifold; under certain additional conditions it is a *Lie group*. All infinite groups in physics are Lie groups, in particular the translation groups, the rotation group, the Galileo group and the Lorentz and Poincaré groups, both to be discussed in the last lecture.

A *(linear) representation* of a group $\mathcal{G}$ in a vector space $\mathcal{V}$ is a homomorphism $\pi : \mathcal{G} \to \mathcal{L}(\mathcal{V})$, $g \mapsto \pi(g)$, where $\mathcal{L}(\mathcal{V})$ is the algebra of linear operators in $\mathcal{V}$, with the properties $\pi(g_1 g_2) = \pi(g_1)\pi(g_2)$ and $\pi(e) = 1$. If $\mathcal{V}$ is a Hilbert space and the $\pi(g)$ unitary, we call π a unitary representation.

Reminder : Lie algebras :

An 'Abstract' Lie algebra is a vector space L, with a bilinear map

$$L \times L \to L, \quad (a, b) \mapsto [a, b],$$

with
1. $[a, b] = -[b, a]$ (anticommutativity)
2. $[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0$ (Jacobi identity)
   for all a,b and c in V.

A Lie group $\mathcal{G}$ has a Lie algebra $\mathcal{L}(\mathcal{G})$. It is the tangent space of $\mathcal{G}$ as a manifold at the point e. Elements of $\mathcal{L}(\mathcal{G})$ can be obtained – roughly – by differentiating 1-parameter groups in $\mathcal{G}$ at the identity element. A representation π of $\mathcal{G}$ gives a (linear) representation $\widehat{\pi}$ of $\mathcal{L}(\mathcal{G})$. If $\mathcal{G}$ is simply connected then π can – in principle – be recovered from $\widehat{\pi}$ by exponentiation

$$\pi(e^{-i\tau h}) = e^{-\tau\widehat{\pi}(h)},$$

for all h in $\mathcal{L}(\mathcal{G})$ and all real τ. If $\mathcal{G}$, together with the representation π, is a symmetry, all operators $\widehat{\pi}(h)$ will commute with time evolution.

Back to physics: The group $\mathcal{G}$ is a symmetry group of a quantum system if there is a unitary representation π of $\mathcal{G}$ in $\mathcal{H}$ with the property that, for all g in $\mathcal{G}$, the operators $\pi(g)$ commute with the

time evolution operators $U(t)$, for all t in R, or equivalently, with the Hamiltonian H.

A Lie algebra $\mathcal{L}(\mathcal{G})$ is an *infinitesimal symmetry* of a quantum system if there is a representation $\widehat{\pi}$ of $\mathcal{L}(\mathcal{G})$ in $\mathcal{H}$, such that, for all h in $\mathcal{L}(\mathcal{G})$, the operators $\widehat{\pi}(h)$ commute with the time evolution operators $U(t)$, for all t in R, or equivalently, with the Hamiltonian operator H.

The great advantage of Lie algebras over Lie groups is that Lie algebras are *linear spaces*. An n-dimensional Lie group $\mathcal{G}$ has an n-dimensional Lie algebra $\mathcal{L}(\mathcal{G})$, in which a basis can be chosen, say $e_1, \ldots e_n$. This simplifies the condition for infinitesimal symmetry to a finite set of linear relations, namely,

$$[\widehat{\pi}(e_j), H] = 0,$$

for $j = 1, \ldots, n$. The $\widehat{\pi}(e_j)$ are usually called the *generators* of the symmetry. Working with Lie algebra generators instead of with the full group is very popular in concrete physical applications of symmetry in quantum theory. Note that the generators are usually unbounded operators, and that therefore some of the above statements should be made more precise by taking into account domain questions. We will not worry about this, as it does not do much harm in practice, at least not in elementary quantum mechanics.

It should finally be remarked that symmetry generators, as observables, are *constants of the motion*. The infinitesimal generators of spatial rotations in a rotation invariant system, for instance with a potential $V(|\vec{x}|)$, are the components of angular momentum, the infinitesimal generators of translation, in a translation invariant system, for instance a 2-particle system with potential $V(\vec{x}_1, \vec{x}_2) = V(\vec{x}_1 - \vec{x}_2)$, are the components of linear momentum. This is another reason why symmetries are important. Some of the best-known constants of motion are connected with symmetry in this way: conservation of linear momentum and angular momentum is a consequence of symmetry under spatial translations and spatial rotations, respectively.

1.15. Concluding remarks

After all this, looking back on our presentation of quantum theory, it seems a good idea to look at the differences between quantum

physics as it emerged in the nineteen twenties and has developed since then, and classical physics, dominant before this period, and still widely used in many applications, where the refinements of quantum theory are irrelevant.

The differences are so deep that one should be surprised that people were able to discover quantum theory.

Let me draw up a list of the most striking differences :

The notion of state of a physical system.

Classical physics: A system of N particles in classical mechanics has R^{6N} as phase space, the space of position and momenta. A state of such a system is just a point in this phase space, a $6N$-tuple $(\vec{p}_1, \ldots, \vec{p}_N, \vec{x}_1, \ldots, \vec{x}_N)$.

Quantum physics: A system of N particles in quantum mechanics is described by an infinite dimensional Hilbert space, the function space $L^2(R^{6N}, d\vec{x}_1, \ldots, d\vec{x}_N)$. States are complex-valued functions from this Hilbert space, wave functions $\psi(\vec{x}_1, \ldots, \vec{x}_N)$

The notion of observables of a physical system.

Classical physics: The observables of an N-particle system are the smooth real functions on the phase space. They can simultaneously be measured and the results predicted with arbitrary precision. A harmonic oscillator, for instance, a particle with mass m moving in 1-dimensional space under the influence of a force pulling it back to the point $x = 0$ with a force proportional to the distance to the origin can have arbitrary positive values for its energy.

Quantum physics: The observables for an N-particle system are self-adjoint operators in the Hilbert space of wave functions. For commensurable observables, with commuting operators, arbitrarily precise simultaneous measurements and predictions are possible. This is not the case for incommensurable observables, with noncommuting operators, on the contrary, there are various restrictions, such as the Heisenberg uncertainty relation for the measurement of position and momentum. The energy of the quantum harmonic oscillator has only discrete energies, namely,

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots,$$

with ω the frequency of the oscillator. Note that the lowest energy is positive; the quantum oscillator has a *ground state* with a *zero point energy* $\epsilon_0 = \frac{1}{2}\hbar\omega$. The hydrogen atom, an electron moving in the attractive Coulomb potential of the nucleus, a system for which no satisfactory classical description could be given, has in its quantum description also a discrete spectrum, corresponding with bound states starting with a ground state, together with a continuous spectrum describing the situation when the electron is no longer bound by the nucleus, but still moves under its influence. Due to external forces, the electron once in a while jumps from one bound state to another, with lower energy. The difference in energy is then emitted as radiation; the possible frequencies precisely the ones predicted by Bohr in 1913.

The notion of time evolution of a physical system.

Classical physics: The states, i.e. points in the phase space R^{6N} move in a flow determined by Newton's equations, brought in Hamiltonian form, as a system of $6N$ first order ordinary differential equations, with now the positions and momenta not in vector notation, but written as $(p_1, \ldots, p_{3N}, x_1, \ldots, x_{3N})$,

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x^j}, \qquad \frac{dx^j}{dt} = \frac{\partial H}{\partial p_j}, \quad j = 1, \ldots, 3N.$$

This system is completely *deterministic* ; if the positions and momenta at an initial time are given, they are, in principle, determined with arbitrary precision at any later time.

Quantum physics: The states in the quantum mechanics for a single particle evolve in time according to the Schrödinger equation

$$\frac{\partial}{\partial t}\psi(\vec{x}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{x}, t) + V(\vec{x})\,\psi(\vec{x}, t).$$

This equation in it self is deterministic; if the wave function is given at an initial time, it can be determined with arbitrary precision for a later time. However, the physics it describes is *nondeterministic*, because knowing the wave function at this later time still leaves us with only a probability for the position of the particle,

1.16. Appendix. More on operators in Hilbert space

1.16.1. Introduction

In this note 'operator' will mean 'linear operator'.
An operator A in a Hilbert space $\mathcal{H}$ is given by two data:

1. its *domain of definition* $\mathcal{D}(A)$,
2. its action $A\psi$, for every ψ in $\mathcal{D}(A)$.

For two operators A and B the identity $A = B$ means:

1. $\mathcal{D}(A) = \mathcal{D}(B)$,
2. $A\psi = B\psi$ for all ψ in $\mathcal{D}(A) = \mathcal{D}(B)$.

For two operators A and B the relation $A \subset B$ means:

1. $\mathcal{D}(A) \subset \mathcal{D}(B)$,
2. $A\psi = B\psi$ for all ψ in $\mathcal{D}(A)$.

One calls B an *extension* of A.

From now on we assume a domain of an operator to be a dense linear subspace of $\mathcal{H}$.

1.16.2. Bounded operators

An operator A is called *bounded* iff

$$\sup_{\psi \in \mathcal{D}(A),\, ||\psi||=1} ||A\psi|| < \infty.$$

This finite supremum is denoted as $||A||$ and called the *norm* of A. A bounded operator has a unique extension to a bounded operator defined on all of $\mathcal{H}$. This extended operator is a *continuous* linear map from $\mathcal{H}$ into itself. From now on if we meet a bounded operator we always shall assume that it is extended to all of $\mathcal{H}$. Because of this the notions 'bounded operator', 'continuous operator' and 'operator defined in all of $\mathcal{H}$' will be synonyms.

From the next section onwards our operators will be unbounded.

1.16.3. Closed operators

Let A be an operator with domain $\mathcal{D}(A)$. The *graph* of A is defined as the collections of couples $(A\psi, \psi)$, for all ψ in $\mathcal{D}(A)$. This collection is a subset of the Cartesian product $\mathcal{H} \times \mathcal{H}$. If it is a closed subset, in the product topology of $\mathcal{H} \times \mathcal{H}$, the A is called a *closed operator*.

If the graph of A is not closed me may close it by adding limit points in the usual way. Two things may happen:

1. The closure of the graph of A is *not* the graph of an operator. We say that A is *not closable*. In this case A is useless for our purpose.

2. The closure of the graph of A is again the graph of an operator, the closure $\overline{A}$. We say that A is a *closable operator*; with $\overline{A}$ the unique closed extension of A. Whenever we meet a closable operator we take its closure, so we may restrict the further discussion to closed operators.

1.16.4. The adjoint of an operator

A bounded operator A has a (bounded) adjoint A^*. To see this we use the well-known theorem that a continuous linear functional $F(\psi)$ on $\mathcal{H}$ can be written as $F(\psi) = (\psi_0, \psi)$, for a unique vector ψ_0. The expression $(\psi_1, A\psi_2)$ is, for a fixed ψ_1 a continuous linear functional $F_{\psi_1}(\psi_2)$. So it can be written as $F_{\psi_1}(\psi_2) = (\psi_1', \psi_2)$. The assignment $\psi_1 \mapsto \psi_1'$ is linear, and defines an operator $\psi_1' = A^*\psi_1$, which is the definition of the *adjoint* A^* *of* A. One easily verifies the properties $(A^*)^* = A$, $(AB)^* = B^*A^*$ and $(\lambda A)^* = \overline{\lambda}A^*$. One has of course the relation

$$(\psi_1, A\psi_2) = (A^*\psi_1, \psi_2), \quad \forall \psi_1, \psi_2 \in \mathcal{H}.$$

For an operator A which is only closable one has a more subtle version of the same argument.

Let A be a closed operator with domain $\mathcal{D}(A)$. One tries to find, for a given vector ψ_1 in $\mathcal{D}(A)$, a vector ψ_1', such that

$$(\psi_1', \psi_2) = (\psi_1, A\psi_2). \quad \forall \psi_2 in \mathcal{D}(A).$$

It is proved in the book mentioned in the reference, on page 252, that there exists a dense linear subspace of $\mathcal{H}$ of such vectors ψ_1. This defines a linear operator that we denotes as A^*, according to $\psi_1' = A^*\psi_1$ and with the domain of vectors ψ_1 just defined. This operator A^* is in fact closed.

Properties: $(A^*)^* = A$, $(\lambda A)^* = \overline{\lambda}A^*$. We cannot say anything about $(AB)^*$ because the product AB may not be defined properly.

Remark: A selfadjoint operator satisfies the relation

$$(A\psi_1, \psi_2) = (\psi_1, A\psi_2), \quad \forall \psi_1, \psi_2 \in \mathcal{D}(A).$$

However, this relation *does not define selfadjointness*. It only states that A is *hermitian (= symmetric)*, which can be expressed as

$$A \subset A^*.$$

For bounded operators selfadjoint = hermitian.

1.17. References

• General physics textbooks on quantum mechanics

There is no shortage of excellent textbooks on quantum mechanics. Here is a personal choice:

[1]. David J. Griffith
Introduction to Quantum Mechanics
Prentice-Hall, 1995.

A good modern introduction; a physics textbook with a more then acceptable level of mathematical precision and rigour.

[2]. Michel Le Bellac
Quantum Physics
Translated from the French. Cambridge University Press, 2006.

This is probably now the best comprehensive general textbook on quantum theory. It is a book for physicists, but its mathematics is careful and modern. It also discusses interesting recent developments.

[3]. Albert Messiah
Quantum Mechanics. Volume I and II
Translated from the French. North-Holland, 1961. Reissued in one volume in 1999 by Dover.

One of the older books that remains valuable because of its thoroughness and clarity of presentation. Well worth having, especially in the moderately priced Dover edition. The original French edition is still available.

[4]. Keith Hannabuss
An Introduction to Quantum Theory
Oxford University Press, 1997

For a mathematics student who wants to know more about quantum mechanics as a physical theory, this lucid book, with its emphasis on mathematical rigour, would be an excellent choice.

[5]. P.A.M. Dirac
The Principles of Quantum Mechanics
Original edition 1930. 4^{th} edition. Cambridge University Press, 1982.

A great classic. In his mathematical thinking Dirac was intuitive – and therefore very non-rigorous, but at the same time imaginative and innovative. His contributions the understanding the underlying mathematical structure of the emerging quantum theory were crucial, even though they had to be put into the rigorous functional analytic framework developed by von Neumann.

• Books on the history of quantum theory

[6]. Jagdish Mehra, Helmut Rechenberg
The Historical Development of Quantum Theory. Volumes 1-6, in 9 parts
Springer, 1982-2000. Reissued in paperback in 2001.

Future research will certainly supply additional material to this monumental history of quantum mechanics from 1900 to 1941 and possibly correct some of its biases, but it will remain unsurpassed in its richness of detail on concepts and persons.

[7]. B.L. van der Waerden
Sources of Quantum Mechanics
North-Holland, 1967. Reissued as a paperback by Dover, 1968.

This book contains seventeen of the most important papers on quantum mechanics from the years 1917-26, in which the theory was developed and formulated, translated into English, together with a 59 page historical introduction.

• Books on the mathematical formalism of quantum theory

[8]. John von Neumann:
Mathematical Foundations of Quantum Mechanics
Princeton University Press 1996.
(Translated from the original 1932 German Springer edition)

A great classic, written by the creator of the mathematical formalism of quantum mechanics. The part on the theory of measurement may have been overtaken by more recent developments, but the general discussion of quantum theory, in particular of selfadjoint operators and the spectral theorem remains instructive and fresh.

[9]. Michael Reed, Barry Simon:
Methods of Mathematical Physics. I: Functional Analysis
Academic Press 1972

This book is an excellent reference for functional analysis, with the theory of operators in Hilbert space as its central topic, especially written for applications in mathematical physics.

[10]. Eduard Prugovecki:
Quantum Mechanics in Hilbert Space. Second Edition
Dover Publications 1981

Even though its general approach may be somewhat dated, it contains a wealth of precise and clearly formulated additional material on the mathematical aspects of quantum theory. The modest price of the Dover edition makes it especially worthwhile.

[11]. Gilbert Helmberg:
Introduction to Spectral Theory in Hilbert Space
North-Holland 1969. Reissued by Dover 2008

A leisurely and clear introduction.

• Internet

- See for a comprehensive list of books on all aspects of quantum theory,

`www.ericweisstein.com/`
`encyclopedias/books/QuantumMechanics.html`

- for short reviews of the history of quantum mechanics,

`www.oberlin.edu/physics/dstyer/StrangeQM/history.html`
`mooni.fccj.org/~ethall/quantum/quant.htm`

• A book on the history of Arabic science

[12]. Ahmed Djebbar
Une histoire de la science arabe
Seuil 2001. 386 p.

Ahmed Djebbar is professor emeritus at the University of Lille in Norther France. He is author or co-author of several authoritive works on the history of Arabic science. This book gives a very readable overview of this subject.

• **Reference added in this revised edition** :

Peter Bongaarts
Quantum Theory. a Mathematical Approach
Springer 2014

This book provides, among other things, a much broader discussion of the topics of this course.

2. Quantum Theory - Many Particle Systems

2.1 Introduction

So far we have discussed single particle systems in quantum mechanics. This lecture will be devoted to general n-particle systems. The mathematical background for this is the theory of n-fold tensor products of Hilbert spaces. This together with its physical meaning will be discussed in the next section. After this, in Section 2.3, attention is focused on the important special case of identical particles. Mathematically this means symmetric and antisymmetric tensor products. A new important quantum phenomenon appears : the existence of bosonic and fermionic particles. The mathematical and physical aspects of this are treated in Section 2.3. The development of the understanding of the physics of identical particles is one of the great stories in the history of quantum mechanics. It is briefly reviewed in Section 2.4.

2.2. Combining quantum systems

New Hilbert spaces can be constructed from given ones. In quantum theory two such constructions play a role, direct sums and tensor products. These two correspond to two different ways of looking at composite quantum systems.

1. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be the Hilbert state spaces of two quantum systems, for instance of two different particles. The system in which both particles do not appear simultaneously, but successively or alternatively, is described by the direct sum $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$. This procedure can be generalized to an arbitrary finite or countably infinite number of Hilbert spaces $\mathcal{H}_j$.

For the Hamitonian operators H_1 and H_2 of the two systems, the Hamiltonian for the composite system is the *sum operator*

$$H = H_1 \oplus H_2,$$

the action of which can be written in terms of column vectors, with elements from $\mathcal{H}_1$ and $\mathcal{H}_2$ as entries, as

$$H \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} H_1\psi_1 \\ H_2\psi_2 \end{pmatrix}.$$

The total Hamiltonian H is then a 2×2 matrix with operators as matrix elements:

$$H = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}.$$

General operators in this direct sum have the form

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

with A_{jk} a linear map from $\mathcal{H}_k$ into $\mathcal{H}_j$. If the Hamiltonian H has the above 'diagonal' form there is no dynamic interaction between the two subsystems; there are no transitions in time. In this case one says that the system has a *selection rule*. Often this is only a first approximation; 'off-diagonal' terms of higher order in an appropriate parameter in the total Hamiltonian will break the selection rule.

It may happen that not only the Hamiltonian but *all* operators that have a physical meaning in $\mathcal{H}_1 \oplus \mathcal{H}_2$ have 'diagonal' form. This would mean, not only that there is no dynamical interaction, but that there is no other meaningful physical relation between the two systems. In general a linear combination of two state vectors represents, after normalization, again a physical state. In this particular case the direct sum Hilbert space $\mathcal{H}_1 \oplus \mathcal{H}_2$ is a mathematical concept only, with no physical meaning, i.e. linear combinations $\lambda_1\psi_1 + \lambda_2\psi_2$, $\psi_1 \in \mathcal{H}_1$, $\psi_2 \in \mathcal{H}_2$, are not physical states. We say that there is a *superselection rule* in $\mathcal{H}$, with the subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ called *superselection subsectors* or *coherent subspaces* of the system. In the next section we shall meet an example of this. The notion of superselection rule was introduced in a paper by Wick and Wightman (Ref.[1]). For a more recent exposition, which takes into account modern developments, see the lecture notes of Fredenhagen, see Ref.[2].

Note that all this goes through for an n-tuple of Hilbert spaces $(\mathcal{H}_1, \ldots, \mathcal{H}_n)$, and, with a few obvious mathematical refinements, for an infinite sequence $(\mathcal{H}_1, \mathcal{H}_2, \ldots)$.

(2.2,a) *Example*: The nucleus of an atom consists of protons and neutrons. These particles have very similar properties, so in nuclear physics one sometimes describes them, in first approximation, as two different states of a single particle, the *nucleon*. The Hilbert space of the nucleon is the direct sum of the Hilbert space of the proton and the Hilbert space of the neutron. In this direct sum Hilbert space

the neutron and the proton are distinguished by 'isobaric spin', a quantum number important in elementary particle physics, in which the word 'spin' has nothing to do with rotations in space like in the case of the spin of an electron.

2. *Tensor products.* Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be the Hilbert spaces of two quantum systems, for instance of two particles *that are assumed to be different.* The Hilbert space of the system in which the particles appear simultaneously is the tensor product space $\mathcal{H}_1 \otimes \mathcal{H}_2$. For quantum system described by an n-tuple of Hilbert spaces $(\mathcal{H}_1, \ldots, \mathcal{H}_n)$ one constructs the tensor product $\mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_n$.

If system 1 has a time evolution operator $U_1(t) = e^{-\frac{i}{\hbar}tH_1}$ with Hamiltonian operator H_1, and system 2 has $U_2(t) = e^{-\frac{i}{\hbar}tH_2}$ with H_2, *and if there is no interaction between the two systems*, then the time evolution of the total system is described by the operator $U(t) = e^{-\frac{i}{\hbar}tH}$, with $U(t)$ the tensor product operator $U_1(t) \otimes U_2(t)$ and total Hamiltonian $H = H_1 \otimes 1_{\mathcal{H}_2} + 1_{\mathcal{H}_1} \otimes H_2$. More interesting is the situation in which the two systems interact. In that case an interaction Hamiltonian H_{12} is added to $H = H_1 + H_2$ and the resulting evolution operator has no longer the form of a 'pure tensor' operator.

(2.2,b) *Example*: The simplest model for the hydrogen atom is that of a particle, an electron, moving in a fixed central potential $V(|\mathbf{r}|)$. The Hilbert space for this system is $\mathcal{H} = L^2(R^3, d\mathbf{r})$. In a slightly more realistic description the hydrogen atom is a two-particle system consisting of the nucleus, a proton with a large mass M and an electron with a small mass m, interacting with each other through the potential $V(|\mathbf{r}_1 - \mathbf{r}_2|)$. The Hilbert space of this 2-particle system is the (completed) tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2 = L^2(R^6, d\mathbf{r}_1 d\mathbf{r}_2)$. Without the interaction the Hamiltonian of this composite system would be the sum of the terms $H_1 \otimes 1_2$ and $1_2 \otimes H_2$, written as H_1 and H_2, with

$$H_1 = -\frac{\hbar^2}{2m}\Delta_1 \ , \quad H_2 = -\frac{\hbar^2}{2M}\Delta_2,$$

in which Δ_j is the Laplace operator in the variable $\mathbf{r}_j$, for $j = 1, 2$. The interaction gives an additional term H_{12} which multiplies the two-particle wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ with $V(|\mathbf{r}_1 - \mathbf{r}_2|)$ and which, as operator, no longer has the form of a pure tensor. Of course, in this particular example the translation invariance of the potential makes

it possible to reduce this picture to a one-particle description, for a single particle with mass $M = \frac{mM}{m+M}$. This description is called the *center of mass* picture.

(2.2,c) *Example*: The Pauli spin model of the hydrogen atom. The state space is the tensor product $L^2(R^3, d\mathbf{r}) \otimes C^2$.

Direct sums of Hilbert spaces were used in this section and the next one for the the notion of 'superselection rule'; tensor products are important in all the sections that follow.

This will be enough on the description of arbitrary systems of two and in general n particles. The remainder of this chapter will be devoted to the important special case of *identical particles*.

2.3. Systems of identical particles

So far all this is not very surprising given the general principles of quantum theory as they have been presented in the preceding lecture. A new and interesting phenomenon occurs for of systems consisting of *identical* particles.

We have argued in lecture 1 that particles in quantum mechanics do not have *orbits* because their position and momentum cannot be measured simultaneously with arbitrary precision. Of course, the probabilities for finding the particles can be concentrated in small disjunct areas of space; however, sooner or later these areas will overlap. All this means that in a system of n identical particles the individual particles cannot be identified. The fact that we cannot observe the difference between the state consisting of a particle (1) concentrated near a point $\mathbf{r}_1$ and a particle (2) near $\mathbf{r}_2$, and a state with particle (1) near $\mathbf{r}_2$ and (2) near $\mathbf{r}_1$, does, strictly speaking, not imply that these two states are the same. However, we take as a fundamental assumption that they are indeed the same. This means, in general, that identical particles in a many-particle system have no 'identity'. A system of n electrons is just that; speaking of a system consisting of electron 1, electron 2, and so on, would not make sense. We add therefore a sixth general axiom to the five formulated in the preceding lecture:

Axiom VI : *In a system of n identical particles, the separate particles have no 'identity'.*

This axiom has important physical consequences, which are typical for quantum theory. All have been verified experimentally. Some will be discussed later. It has also consequences for the mathematical description of quantum systems. To these we turn now.

Start, for the description of a system of n identical particles, each on its own in a 1-particle Hilbert space $\mathcal{H}^{(1)}$, with the n-fold tensor product space $\otimes^n\mathcal{H}^{(1)}$. According to Axiom VI the unit vector $\psi_1 \otimes \ldots \otimes \psi_n$ in $\otimes_{j=1}^n \mathcal{H}^{(1)}$ represents the same physical state as the permuted vector $\psi_{\sigma(1)} \otimes \ldots \otimes \psi_{\sigma(n)}$, for a permutation σ of the indices $1, 2, \ldots, n$. The map $\psi_1 \otimes \ldots \otimes \psi_n \mapsto \psi_{\sigma(1)} \otimes \ldots \otimes \psi_{\sigma(n)}$ defines in $\otimes_{j=1}^n \mathcal{H}^{(1)}$ by linear extension a representation $\{P(\sigma)\}_\sigma$ of the *symmetric group* S_n, the group of permutations of n objects. This is a finite group; as such its irreducible representations are finite dimensional, and are – or are equivalent to – unitary representations. The number of its inequivalent irreducible representations is finite. Its representations are completely reducible, which means that a general representation can be written as a direct sum of irreducible ones. The properties of S_n and its representations are discussed in the book by Sagan (Ref.[3]).

The Hilbert space $\otimes^n\mathcal{H}^{(1)}$ can, as a consequence of these properties, be written as a finite direct sum of Hilbert subspaces

$$\otimes^n\mathcal{H}^{(1)} = \mathcal{H}_{j_1} \oplus \ldots \oplus \mathcal{H}_{j_p}.$$

Each of the spaces $\mathcal{H}_{j_k}$ carries an in general infinite direct sum of (finite dimensional) unitary irreducible representations of the permutation group S_n, with the representations in different $\mathcal{H}_{j_k}$ mutually inequivalent. The representing operators $U(\sigma)$ have, in the above direct sum realization of $\otimes^n\mathcal{H}^{(1)}$, the form

$$U(\sigma) = \begin{pmatrix} U_{j_1}(\sigma) & 0 & \cdot & \cdot \\ 0 & U_{j_2}(\sigma) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & U_{j_p}(\sigma) \end{pmatrix}.$$

Two vectors ϕ_1 and ϕ_2 in $\otimes^n\mathcal{H}^{(1)}$ with $\phi_2 = U(\sigma)\phi_1$, for some $\sigma \in S_n$, are equivalent as physical states. An operator A in $\otimes^n\mathcal{H}^{(1)}$ is admissable as a physical operator only if the images $A\phi_1$ and $A\phi_2$ are also equivalent. This leads to the general requirement that admissable operators have to commute with all $U(\sigma)$. This means that,

following an appropriate version of Schur's lemma, that physical operators also have the diagonal form

$$A = \begin{pmatrix} A_{j_1} & 0 & \cdot & \cdot \\ 0 & A_{j_2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & A_{j_p} \end{pmatrix}.$$

This is the situation we discussed in the preceding section: a superselection rule, with in the Hilbert space $\otimes^n \mathcal{H}^{(1)}$ the subspaces $\mathcal{H}_{j_k}$ as the superselection subsectors. There is no interaction between the $\mathcal{H}_{j_k}$. The space $\otimes^n \mathcal{H}^{(1)}$ is a purely mathematical construction and has in itself no physical meaning. The subspaces $\mathcal{H}_{j_k}$ represent physical systems, each describing an n-particles system consisting of different kind of particles.

Consider first the simplest nontrivial example: that of a 2-particle system. The group S_2 has two inequivalent irreducible representations. See for this Ref.[3]. The space $\otimes^2 \mathcal{H}^{(1)}$ is a direct sum $\mathcal{H}_s \oplus \mathcal{H}_a$, of the subspaces determined by the projection operators defined by linear extension of

$$P_s(\psi_1 \otimes \psi_2) = \frac{1}{2}[(\psi_1 \otimes \psi_2) + (\psi_2 \otimes \psi_1)]$$

and

$$P_a(\psi_1 \otimes \phi_2) = \frac{1}{2}[(\psi_1 \otimes \psi_2) - (\psi_2 \otimes \psi_1)].$$

This means that we have two pairs of particles of an intrinsically different type. The first are called *bosonic particles*, or *bosons* for short, the second *fermionic particles* or *fermions*.

The image spaces of the projection operators P_s and P_a are naturally isomorphic to the symmetric and antisymmetric tensor product spaces $\mathcal{H}^{(1)} \otimes_s \mathcal{H}^{(1)}$ and $\mathcal{H}^{(1)} \otimes_a \mathcal{H}^{(1)}$.

Consider next a system of three or more identical particles. The permutation group S_n has for every $n > 2$ as irreducible representations in the first place again those in the symmetric and completely antisymmetric tensor product spaces $\otimes_s^n \mathcal{H}^{(1)}$ and $\otimes_a^n \mathcal{H}^{(1)}$, but new representations of mixed symmetry type appear. Do these additional representations correspond to additional types of particles?

Bosons and fermions can be easily distinguished experimentally by their physical properties which follow from the theory as discussed

here. It is mainly a matter of a different counting of states. These properties are intrinsic properties of the particles, which do not depend on whether they belong to a two-particle system or a to a system of more than two particles. From this we may infer that the mixed symmetry representations of S_n have no physical meaning in the context of the theory of indentical particles. So we assume that there exists only bosons and fermions, as is confirmed by the fact that no other types of particles have ever been observed.

There is another important physical difference between bosons and fermions, based on a simple but deep connection with spin:

It is an experimentally observed general fact that all particles with integer spin are bosons; all particles with half integer spin are fermions.

So far there is in (non-relativistic) quantum theory no proof for the the connection between spin and statistics, even though the experimental status is completely unambiguous. In the wider context of relativistic quantum theory, in particular relativistic quantum field theory, a topic that will briefly touched upon in 14, it is possible to prove a general *spin-statistics theorem*. See for instance the book of Streater and Wightman (Ref.[4]).

Note that in all this one may read 'states' for 'particles'. An electron has spin 1/2 and is therefore a fermion. According to the rules for composing spins, the state space of a system of two electrons is the direct sum of a spin 0 and a spin 1 space, so this system is a boson state.

All this enables us to formulate as a general principle, as a consequence of Axiom VI – maybe with the additional assumption of the connection between spin and statistics for elementary non-relativistic quantum mechanics :

In quantum theory a composite system made up from n identical systems with each the same Hilbert space $\mathcal{H}$ has as state space either the symmetric tensor product $\otimes_s^n\mathcal{H}$ (a bosonic system) or the antisymmetric tensor product $\otimes_a^n\mathcal{H}$ (a fermionic system). Moreover, boson states have integer and fermion states half-integer spin.

2.4. Historical remarks

The historical development of the complex of scientific notions discussed in the preceding sections is that of a piecemeal and fragmentary discovery of at first unrelated facts and ideas, not unlike

the earlier the development of quantum mechanics itself. One is reminded of an archeological excavation, in which one first discovers fragments of brickwork, than realizes that these are pieces of complete walls. In the end, if one is lucky, one may obtain one single picture of a complete city.

Looking backwards it is easy, with the knowledge and understanding that we have now, to describe the development in the opposite direction, starting with the fundamental fact that quantum particles do not have an identity, suggested by Heisenberg's uncertainty relations, and formulated as Axiom VI, and then derive from this the full theory, possibly with assuming in addition the spin-statitics relation for elementary quantum mechanics. The picture thus obtained is in the end conceptually more satisfying than the sequence of historical events, interesting as they are in themselves. A few words about this history will make this clear.

The context of quantum mechanics in the period, say, from 1925 till 1929, when the elements of the description of systems of identical particles were formulated, was the physics of atoms. In this the picture was that of an atom consisting of a central nucleus with its surrounding electrons, together with the manner in which atoms interact to form molecules. What was experimentally observed were atomic and molecular spectra.

The story starts with Pauli's discovery that looking at atomic spectra, in particular those of the helium atom, one finds that certain specific energy levels are missing, in a very systematic way. This led him in 1925 to the formulation of his *exclusion principle* – for which he later, in 1945, received the Nobel prize – stating, roughly, that two electrons cannot occupy the same state. It was immediately clear that this had important consequences; without it the periodic systems of elements would look very different. Pauli also noted that the electron seemed to have an additional quantum number but he left it at that. The Dutch physicists Goudsmit and Uhlenbeck identified this shortly afterwards as an intrinsic angular momentum; the *spin* of the electron.

Up to this point the only elementary particles known were electrons. In nuclear physics as it emerged somewhat later new particles were found which did not satisfy the exclusion principle, for instance, π-mesons, unstable spin 0 particles found in cosmic radiation and

later produced in particle accelerators. From this it became clear that there exist in nature two distinct types of particles, those with integer spin, bosons, and those with half-integer spin, fermions, with important consequences, in particular for quantum statistical mechanics, where Fermi-Dirac statistics takes the place of the statistics of Maxwell-Boltzmann in classical statistical mechanics.

So historically speaking, Pauli's exclusion principle is the basic fact in the description of systems of identical particles from which everything else later followed. But looking backwards it is clear that the theoretical starting point in this is the principle that particles in quantum theory have no 'identity' (Axiom VI). The exclusion principle is a simple consequence of this.

2.5. References

[1]. G.C. Wick, A.S. Wightman, E.P. Wigner
The Intrinsic Parity of Elementary Particles
Physical Review 88, 101-105 (1952)

Available at:
`http://dieumsnh.qfb.umich.mx/archivoshistoricosMQ/ModernaHist/Wick.pdf`

This is the basic reference for this topic. All later papers refer to it.

[2]. Klaus Fredenhagen
Superselection Sectors
Notes from Lectures held at Hamburg University 1994/1995

Available at
`www.desy.de/uni-th/lqp/psfiles/superselect.ps.gz`

[3]. Bruce A. Sagan
The Symmetric Group. Representations, combinatorical Algorithms, and Symmetric Functions. Second Edition
Springer 2001

[4]. Raymond F. Streater, Arthur S. Wightman
PCT, Spin and Statistics, and All That
Princeton University Press 2000

3. Quantum Theory - Quantum Statistical Mechanics

3.1. The classical case

In the preceding lecture we discussed the quantum mechanics of systems of n particles, a description in which we still looked at the properties of the separate particles. For very large systems systems the description of the individual particles no longer makes sense. Think of a gas in a container. For such a system, with something like 10^{25} particles in a cubic centimeter, it is in principle possible to study the behaviour of the individual particles, but only very much in principle, because it would be extremely difficult and complicated. But above all, it would be totally uninteresting. What is of interest for such systems are overall properties, pressure, temperature, in general what one calls *'thermodynamic"* properties.

Let us start with a few historical remarks. First thermodynamics. Thermodynamics, as a theoretical science describing the macroscopic properties of matter, gases, liquids and solids, as an engineering science for the understanding of the working of steam engines, with as principal notions temperature, pressure and work, was invented in the eighteenth century (Carnot), further developed (Clausius) and given its final form, which is still with us (Planck) in the nineteenth century.

All this without having in mind an underlying microscopic picture of matter, as most physicists and philosophers at that time did not believe in the reality of atoms. During the second half of the nineteenth century this changed; more and more physicists began to take serious an underlying picture of moving and interacting atoms. The great challenge then became to derive the macroscopic laws of thermodynamics from the microscopic laws which according to Newton's classical mechanics were assumed to govern the motions of these atoms. One realized that this derivation of macroscopic properties from microscopic ones would involve statistical methods to calculate the macroscopic properties as mean values.

Beginning in the second half of the nineteenth century a *statistical description* of this type was developed. Pioneers were James Clark Maxwell, Josiah Willard Gibbs, the first American theoretical physicist to become known in the rest of the world, and Ludwig

Boltzmann. They created what is now known as *classical statistical mechanics*, the theory of the collective behaviour of large assemblies of small subsystems, based on probabilistic arguments.

The basic concept of classical statistical mechanics is that of a probability distribution on phase space, a so-called *ensemble*, which is used to calculate mean values of the system as a whole, such as mean energy and pressure. Note that the term 'ensemble' was coined by Gibbs, this before probability theory was given its modern mathematical formulation by Kolmogorov in nineteen twenties. The word 'ensemble' has survived this more modern formulation as an anachronism in physics textbooks, where one finds talk of "a cloud of identical systems moving through phase space", a rather primitive way of expressing the main notion of probability theory, which I believe has confused generations of students. See for critical remarks on this Ref.[6].

It took some time to find out which ensembles should be used. *Ergodic theory*, the study of the behavior of dynamical systems for long times, was developed for this. Important theorems in it were proved by von Neumann and Birkhoff. By the way, ergodic theory is another example of a mathematical theory which started as a part of physics and later developed into an independent part of pure mathematics, becoming the general theory of the asymptotic behavior of 1-parameter groups of measure preserving transformations. An interesting field of mathematics, but no longer relevant to physics.

All this led to the various ensembles that are now used in statistical mechanics, depending on the situation in which a system is observed. All of these are *stationary ensembles* for systems in equilibrium. Note that in an equilibrium situation the points of phase space that represent the various possible states of the system move through phase space, but that the ensemble, the probability distributions remains the same. Helpful in this was *Liouville's theorem* stating that the basic $6N$-form of the phase space as a symplectic manifold is invariant under time evolution. The motion of the particles is represented by a *flow*, the flow determined by the Hamiltonian vector field, given by the Hamilitonian function of the system. "The phase liquid is incompressible under the motion in time."

The first and in a certain way basic ensemble was the *micro canonical ensemble*, for an isolated system, for which the total energy is constant. One restricts the phase space, usually denoted as Γ, to the submanifold of dimension $3N-1$, given by $H(\mathbf{p},\mathbf{q}) = \mathbf{E_0}$, for a given value E_0 of the total energy, or to a very thin 'energy shell' around this value. One then uses Liouville's theorem together with the assumption that the so-called *ergodic theorem* is valid, meaning that "phase averages are equal to time averages", to conclude that equal parts of the energy surface (or equal volumes in the energy shell) should be given equal a priori probabilities.

The next ensemble, more or less derived from the micro canonical ensemble, is the *canonical ensemble* or *Gibbs ensemble*. It describes a system in a 'heat bath', i.e. the system is enclosed in a very large box with a fixed temperature T, in such way that no particles can enter or leave the system, while still energy with this surrounding 'heat bath' can be exchanged. It is the most important and most widely used ensemble. Note in passing that the original goal of deriving the thermodynamics from the microscopic picture of matter, i.e. deriving the ensembles of statistical mechanics from the classical mechanics of the atoms, has only very partially been reached. Many of the derivations are nonrigorous or incomplete. The ergodic theorem, for instance, has only been proven for a very restricted class of mechanical systems. (System of billiard balls, Sinai). Nevertheless, statistical mechanics whether rigorously derived from first principles or not, is a very successful physical theory and has become generally accepted.

The canonical ensemble has a probability density

$$\rho_\beta(\mathbf{p},\mathbf{q}) = \frac{1}{Z(\beta,V,N)} e^{-\beta H(\mathbf{p},\mathbf{q})},$$

with $\mathbf{p} = (\vec{p}_1,\ldots,\vec{p}_N)$ and $\mathbf{q} = (\vec{q}_1,\ldots,\vec{q}_N)$, the momentum and position variables in the classical phase space Γ. N is the (extremely large) number of particles of the system, V its volume and $\beta = 1/k_B T$, with k_B the constant of Boltzmann, a constant of nature, and T the (absolute) temperature. Because ρ is a probability density, integrating it over the phase space Γ should give unity. For this we have as normalization factor the expression in the numera-

tor, the so-called *canonical partition function*

$$Z(\beta, V, N) = \int_{\Gamma} e^{-\beta H(\mathbf{p},\mathbf{q})} d\mathbf{p}\, d\mathbf{q}.$$

Averages of a physical observable, for instance the energy H, is then given by the integral

$$< H >_{\rho_\beta} = \int_{\Gamma} H(\mathbf{p}, \mathbf{q})\, \rho_\beta(\mathbf{p}, \mathbf{q})\, d\mathbf{p}\, d\mathbf{q}.$$

From Z the macroscopic and thermodynamical properties of the system can be derived. For a system of free particles it is not hard to calculate Z. The difficult problem in classical statistical mechanics in general is to do this for a Hamiltonian function H of a system of interacting particles. There are other ensembles, for example the *microcanonical ensemble* for a totally isolated system, with no interaction whatsoever with the outside world and the *grandcanonical ensemble* for systems that both energy and matter exchange with a larger outside system. This is enough about classical statistical mechanics for our purpose, so on to quantum statistical physics.

3.2. The quantum case

What we know about the fundamentals of gases – kinetic theory, the relations between pressure and temperature, van der Waals' theory of molecular interactions, is based on classical statistical mechanics. For more general, and in particular more recent subjects we need a quantum version of statistical mechanics. Note that Planck's calculation of the energy spectrum of black-body radiation, which stood right at the beginning of quantum theory, can – with hindsight – be seen as an application of quantum statistical mechanics 'avant la lettre'.

More modern developments in phyiscs such as solid-state and condensed matter physics, the theory of metals, semiconductors, phase transitions, and, for instance, a large part of molecular physics and astrophysics, can only be understood properly by quantum statistical physics. This is in particular true for such a recent topics as superfluidity, and superconductivity, all purely quantum phenomena.

As we have seen, quantum theory, quantum mechanics, is in its essence a probabilistic theory. Quantum statistical mechanics adds

an additional layer of probability ideas to this. The first question to be asked is: "What is a quantum ensemble?" The answer is :

An ensemble in quantum statistical physics is a density operator*, i.e. a positive selfadjoint trace class operator $\widehat{\rho}$ in the Hilbert space $\mathcal{H}$ of the quantum system, with trace equal to one.*

Reminder: A bounded operator A in a Hilbert space $\mathcal{H}$ is called a *trace class operator* iff for an orthonormal basis $\{\varphi_n\}_n$

$$\sum_n |(\varphi_n, A\varphi_n)| < \infty.$$

If this holds for one orthonormal basis, it will hold for all others. One then defines

$$\mathrm{Tr}\,(A) = \sum_n (\varphi_n, A\varphi_n),$$

as the *trace* of A. This number is independent of the choice of basis. The product of two trace class operators is trace class. For two such operators A and B one has

$$\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA),$$

as in finite dimensional linear algebra. A trace class operator has a purely discrete spectrum. Note that every linear operator in a finite dimensional vector space has a trace; but in an infinite dimensional Hilbert space not even all bounded operators are trace class.

The next question is: "How does one calculate averages with such a quantum ensemble?" The answer is:

The average of an observable represented by a selfadjoint operator A with respect to a quantum ensemble, represented by a density operator $\widehat{\rho}$ is equal to

$$< A >_{\widehat{\rho}} = \mathrm{Tr}\,(\widehat{\rho}A).$$

For this prescription to make sense the product $\widehat{\rho}A$ has to be a trace class operator. The observable A cannot be an arbitrary bounded operator, but has to satisfy a restriction. It does not need to be trace class; it is should be *completely continuous*, a weaker property than trace class. For the sake of completeness, here is the definition: An operator is called *completely continuous* or *compact* iff the image of every bounded set has compact closure. We shall not need this definition here.

At this point one might ask how one ever got the idea of representing a state in quantum statistical mechanics by a density operator. We asked the same question for representing a state in quantum mechanics by a vector in a Hilbert space. There the answer was historic, a matter of a gradual development of ideas which finally resulted in the idea of using Hilbert space notions. Here the answer is simpler. A state should assign in a linear way numbers (mean values) to all operators, i.e. it should be a *linear functional* on the linear space of the operators in the Hilbert space $\mathcal{H}$. For a finite dimensional Hilbert space one easily derives that a linear functional $F(A)$ on the (finite dimensional) linear space of operators can be written as $F(A) = \mathrm{Tr}(\widehat{\rho}A)$, for a unique operator $\widehat{\rho}$. A state should be *real*, i.e. give real numbers for selfadjoint operators, *positive*, i.e. give positive numbers on positive operators, and normalized, i.e. should give 1 on the unit operator. The consequence of these additional requirements is that $\widehat{\rho}$ must be positive, selfadjoint and have trace equal to 1. Every operator in a finite dimensional space is of course trace class. In the case of an infinite dimensional Hilbert space not all operators are trace class, not even the bounded operators, so there we have to add the property of $\widehat{\rho}$ being trace class. This general argument, leading to the definition of what a state is in quantum statistical mechanics was already given in 1930 by von Neumann in his book on the foundations of quantum theory.

Finally: "What density operator $\widehat{\rho}$ corresponds with the canonical ensemble ρ_β?" The answer is

$$\widehat{\rho}_\beta = \frac{1}{Z^{\mathrm{qu}}(\beta, V, N)}\, e^{-\beta \widehat{H}},$$

with for the normalization the quantum partition function $Z^{\mathrm{qu}}(\beta, V, N)$ with

$$Z^{\mathrm{qu}}(\beta, V, N) = \mathrm{Tr}\,(e^{\beta \widehat{H}}).$$

The quantum partition function is again the quantity from which the macroscopic and thermodynamic properties are derived. Note in passing that integration in the classical case has become the taking of a trace in an analogous way. This is typical; taking a trace may quite generally be seen as 'noncommutative integration'.

What happened with the notion of state vector, so crucial in our axiom system for quantum theory that we explained in the first

part of this lecture? It seems to have disappeared altogether. What happened is that we have generalized the notion of *state*, in fact generalized our system of axioms, without saying so explicitly. We turn now to an explicit formulation of a second version of our system of axioms for quantum theory.

3.3. A second axiom system for quantum theory

In our first lecture we gave the simplest version of an axiom system for quantum theory; we called it 'Version 1'. We now present 'Version 2'.

The main concepts in 'Version 1' were

state,

observable,

rule for physical interpretation which connects these two,

dynamics,

symmetries.

All this returns in the new system, with however a new or generalized notion of *state*.

We start with a Hilbert space $\mathcal{H}$. It is still there, but no longer as the space of state vectors, but as a background object. We then state five axioms, generalizing the five axioms of "Version 1".

• **States**

Axiom I′: *A state of a quantum system is represented by a selfadjoint positive trace class operator with trace* 1.

The space of states will be denoted $\mathcal{S}$. It is a selfadjoint subset of $B(\mathcal{H})$, the complex linear space of all bounded operators in $B(\mathcal{H})$.

Let $\widehat{\rho}_1$ and $\widehat{\rho}_2$ be two different elements of $\mathcal{S}$, and let λ be a real number with $0 < \lambda < 1$. It is not hard to show that the sum $\lambda\widehat{\rho}_1 + (1-\lambda)\widehat{\rho}_2$ is again an element of $\mathcal{S}$. This result means that $\mathcal{S}$ is a *convex* set.

Reminder: A convex set is a subset $\mathcal{C}$ of a vector space V with the property

$$a_1, a_2 \in \mathcal{C} \;\rightarrow\; a = \lambda a_1 + (1-\lambda)a_2 \in \mathcal{C}, \;\; 0 \leq \lambda \leq 1$$

The element a is called a *convex linear combination* of a_1 and a_2. It is a trivial combination for $\lambda = 0$, for $\lambda = 1$, or for $a_1 = a_2$. If a cannot be written as a nontrivial convex combination it is called an extremal point, otherwise a nonextremal point. This is because any two elements a_1 and a_2, with $a_1 \neq a_2$, give a line segment in $\mathcal{C}$ consisting of the elements $a = \lambda a_1 + (1 - \lambda)a_2$, for all $0 \leq \lambda \leq 1$. The set $\mathcal{C}$ is clearly a disjunct union of a 'boundary' and an 'interior'. These notions of 'interior' and 'boundary' have not the usual topological meaning, as a convex set does not necessarily have a topology.

In quantum theory the convex set $\mathcal{S}$ of states, the extremal or 'boundary' elements are called *pure states*, the nonextreme or 'interior elements' are called *mixed states*. The reason for this will become clear further in this lecture.

Important theorem: *A density operator $\widehat{\rho}$ is a pure state if and only if $\widehat{\rho}$ is a one-dimensional projection operator.*

The proof of this theorem follows from the following argument:

A density operator has as a trace class operator a purely discrete spectrum. The spectral theorem has therefore the simple 'finite dimensional' form

$$\widehat{\rho} = \sum_j \lambda_j E_j,$$

with positive eigenvalues λ_j, all with finite multiplicity, and with

$$\sum_j \lambda_j = 1,$$

and with each E_j a 1-dimensional projection operator. Suppose the set of eigenvalues is larger than one. Let us divide the set of eigenvalues into two nonempty disjoint sets, $\{\mu_s\}_s$ and $\{\nu_t\}_t$, possible because there are at least two eigenvalues λ_j. Call $\sum_s \mu_s = \mu$ and $\sum_t \nu_t = \nu$. Both are positive number; we have $\mu + \nu = 1$. Define

$$\widehat{\rho}_1 = \frac{1}{\mu} \sum_s \mu_s E_s, \qquad \widehat{\rho}_2 = \frac{1}{\nu} \sum_t \nu_t E_t.$$

Both expressions define states. It is clear that $\mu\widehat{\rho}_1 + \nu\widehat{\rho}_2 = \widehat{\rho}$, and as a nontrivial convex linear combination of the two states $\widehat{\rho}_1$ and $\widehat{\rho}_2$, it is a mixed state. If there is only one eigenvalue, say λ_1, which must

necessarily be equal to 1, the spectral theorem reduces to $\widehat{\rho} = E_1$, i.e. $\widehat{\rho}$ is a pure state. This proves the theorem.

• **Observables**

Axiom II′: *The observables of a quantum system are represented by the selfadjoint operators in* $\mathcal{H}$.

This is the same as in 'Version 1'. No further comments are required.

• **The relation between I′ and II′. Physical interpretation**

Axiom III′: *If the system is in a state represented by a density operator* $\widehat{\rho}$*, then the probability distribution function for the outcome of the measurement of an observable* A *is*

$$F_{\widehat{\rho}}(\alpha) = \mathrm{Tr}\,(\widehat{\rho}E_\alpha),$$

with the E_α the spectral projections of A. *For* n *commensurable observables* $A_1, \ldots, A_n$ *the joint distribution function is*

$$F_{\widehat{\rho}}(\alpha_1, \ldots, \alpha_n) = \mathrm{Tr}\,(\widehat{\rho}E_{\alpha_1,\ldots,\alpha_n}),$$

with $E_{\alpha_1,\ldots,\alpha_n}$ *the projections from the* n*-parameter spectral resolution of the sequence of commuting selfadjoint operators* $\{A_j\}_j$.

The result, a distribution function, in one variable for a single observable, and in n variable for a system of n commensurable ones, is very much the same as in 'Version 1'. To see the difference, and the relation with Axiom III from 'Version 1' we use the theorem about pure and mixed states. The average or expectation value for the measurement of an observable represented by a selfadjoint operator A in a state $\widehat{\rho}$ is, as was already discussed, $< A >_{\widehat{\rho}} = \mathrm{Tr}\,(\widehat{\rho}A)$.

Let $\widehat{\rho}$ be a pure state, then according to the theorem it can be written as $\widehat{\rho} = E_\psi$, with E_ψ the projection on the unit vector ψ. Choose an orthonormal basis, with ψ as the first vector, i.e. an orthonormal sequence $(\psi, \psi_2, \psi_3, \ldots)$. Using the idempotency property $E_\psi^2 = E_\psi$ and the trace formula $\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA)$, the average of A in $\widehat{\rho}$ becomes

$$< A >_{\widehat{\rho}} = \mathrm{Tr}\,(\widehat{\rho}A) = \mathrm{Tr}\,(E_\psi A) =$$
$$= \mathrm{Tr}\,(E_\psi^2 A) = \mathrm{Tr}\,(E_\psi A E_\psi) = \sum_j (\psi_j, E_\psi A E_\psi \psi_j) =$$
$$= \sum_j (E_\psi \psi_j, A E_\psi \psi_j) = (E_\psi \psi, A E_\psi \psi) = (\psi, A\psi),$$

which is exactly the formula for the average in a state vector ψ, as it followed from Axiom III.

For a pure state the full Axiom III$'$ reduces in a similar way to the full Axiom III from 'Version1'.

• **Time evolution**

Axiom IV$'$: *The time evolution of a quantum system is described by a strongly continuous* 1*-parameter group of unitary operators* $\{U(t)\}_t$ *which acts on the density operator* $\widehat{\rho}$ *as*

$$\widehat{\rho} \to U(t)\widehat{\rho}U(t)^{-1} = e^{\frac{i}{\hbar}t\widehat{H}}\widehat{\rho}\, e^{-\frac{i}{\hbar}t\widehat{H}}.$$

• **Symmetries**

Axiom V$'$: *A symmetry of the system, given by a unitary operator* U*, or by a group of unitary operators representing a group* $\mathcal{G}$ $\{U(g)\}_{g\in\mathcal{G}}$ *is described by an action on the state* $\widehat{\rho}$ *as*

$$\widehat{\rho} \to U\widehat{\rho}U^{-1}, \qquad \widehat{\rho} \to U(g)\widehat{\rho}U(g)^{-1}.$$

These two axioms reduce to Axiom IV and V for the case of a pure state $\widehat{\rho} = E_\psi$, as can be derived easily.

Final remark: The two axiom systems 'Version 1' and 'Version 2' are both standard tools in physics. They cover almost everything that one needs in quantum theory. There are however situations for which this not – or not quite – the case:

Phase transitions: For a system of gas, liquid and solid matter there are, when external parameters are changed, discontinuous changes in the value of macroscopic quantities, *phase transitions*. Statistical mechanics, both classical and quantum, which describe systems consisting of a finite number of particles, in other word with a finite number of degrees of freedom, very large but still finite, lead to analytic expressions, smooth functions, without the discontinuities that are typical of phase transitions. There are two ways to get these discontinuities.

The first is to take the limit for the number of particles going to infinity, *in the numerical results* of the finite theory, because the limit of a sequence of smooth functions may have discontinuities.

The second is to create a theory of classical and quantum statistical mechanics directly for infinite systems. This will involve a new version of our axioms.

Quantum field theory: Quantum fields are systems with an infinite number of degrees of freedom. In a very simple way they can be seen as infinite collections of harmonic oscillators. We shall provide a short introduction to quantum field theory in our last lecture. To set up a mathematically rigorous framework for quantum field theory a description as an infinite system is unavoidable.

Conclusion: A third version of an axiom system for quantum theory is useful for the description of phase transitions; it is necessary for a rigorous discussion of quantum field theory. So in the next lecture we shall sketch an axiom system 'Version 3'.

3.4. References

[1]. Roger Balian
From Microphysics to Macrophysics,
Methods and Applications to Macrophysics. I, II
Springer 2007

[2]. Carolyne Van Vliet
Equilibrium and Non-Equilibrium Statistical Mechanics
World Scientific 2008

Two of the many excellent and comprehensive modern textbooks on thermodynamics and statistical mechanics, classical as well as quantum.

[3]. Paul and Tatjana Ehrenfest
The Conceptual Foundations of the Statistical Approach in Mechanics
Dover 1990

An English translation of *Begriffliche Grundlagen der statistischen Auffassung in der Mechanik*, published in 1912 in one of the volumes of the *Enzyclopädie der mathematischen Wissenschaften.* A classic.

[4]. G. Gallavotti
Statistical Mechanics. A Short Treatise
Springer-Verlag 1999

A mathematically rigorous exposition of classical and quantum statistical mechanics. An internet version can be downloaded at :

http://www.eknigu.org/get/P_Physics/
PT_Thermodynamics,%20statistical%20physics/
Gallavotti.%20Statistical%20
mechanics%20(1999)(359s).pdf

[5]. Josiah Willard Gibbs
Elementary Principles in Statistical Mechanics:
Developed with special reference to the rational foundation of thermodynamics
Dover 1960.

The original edition was published in 1902 and can be found at :

ftp://ftp.bnf.fr/009/N0099748_PDF_1_-1DM.pdf

A classic text, still worth reading

[6]. A.I. Khinchin
Mathematical Foundations of Statistical Mechanics
Original Russians edition 1943. English translation. Dover 1949

The first serious discussion of the mathematical foundations of classical statistical mechanics and still the best in what we call the Boltzmann approach. The probabilist J.L. Doob wrote: "[Khinchin] shows how to make classical statistical mechanics a respectable rigorous discipline, with a consistent mathematical content." Note Khinchin's severe criticism of the lack of mathematical rigour in discussions on statistical mechanics by physicists in the preface and the first introductory chapter. These can be found separately at :

http//:www.gap-system.org/~history/Extras/
Khinchin_preface.html

http://www.gap-system.org/~history/Extras/
Khinchin_introduction.html

[7]. R. Jancel
Foundations of Classical and Quantum Statistical Mechanics
Translated from the 1963 French edition
Pergamon 1969

4. Physical Theories as Algebraic Systems

4.1. Introduction

This lecture is somewhat different from the others. It is more mathematical. It also contains less standard material, but discusses ideas that have been floating around in the literature for some time and which I have assembled into a single framework. Many details are still missing. In any case the general picture that I shall put forward in this lecture is more important than those details.

The content of this lecture is, apart from generalities, independent from the rest of the lectures. A bit more mathematical knowledge is needed, the outlines of which I shall try to supply.

It is in principle possible to describe both quantum and classical physics within a single algebraic framework. In such a formulation physical systems appear as 'algebraic dynamical systems'.

Let me immediately start with giving a provisional and, admittedly, rather rough definition:

An *algebraic dynamical system* will be a couple

$$(\mathcal{A}, \{\phi(t)\}_{t\in R^1})$$

in which $\mathcal{A}$ is an associative complex $*$-algebra with unit element, and $\{\phi(t)\}_{t\in R^1}$ a 1-parameter group of $*$-automorphisms of $\mathcal{A}$.

The states of such a system are elements of the collections of positive normalized linear functionals on $\mathcal{A}$. Symmetries are represented by $*$-automorphisms, or groups of such automorphisms that commute with the ϕ_t. The elements of $\mathcal{A}$ are the observables, the automorphisms ϕ_t describe the time evolution, the expression $\omega(A)$ for a linear functional ω and an observable A give the average value of the observable A in a state ω. Physicists call this the 'expectation value'; probabilists call it 'expected value'. Higher moments are given by $\omega(A^2)$, $\omega(A^3)$, etc..

Remark: The above definition applies to nonrelativistic physics, to which most of these lectures are devoted. In nonrelativistic physics time is an external parameter. This is not the case in relativity theory. There time has no separate meaning; it is part of 4-dimensional

spacetime. Instead of algebraic dynamical system we have there *algebraic covariance systems*, couples

$$(\mathcal{A}, \phi(\Lambda, a)_{(\Lambda,a)\in\mathcal{P}})$$

with the $\phi(\Lambda, a)_{(\Lambda,a)}$ $*$-automorphisms of $\mathcal{A}$, which represent the Poincaré group $\mathcal{P}$, the inhomogeneous Lorentz group. In this situation the notions of time evolution and symmetery, at least spacetime symmetry, coincide. All this will be explained in the last lecture.

We distinguish two cases:

1. The algebra $\mathcal{A}$ is *commutative*: *classical physics.*
2. The algebra $\mathcal{A}$ is *noncommutative*: *quantum physics.*

This distinction is the most important point of this lecture, as will become clear.

Historical remark: It was in quantum theory that an algebraic point of view of the sort that we have in mind first appeared. The mathematical basis of quantum theory is the use of operators in Hilbert space, as we have already explained in detail in Lecture 1; from studying such operators it is only one step to the study of *algebras of operators.*

Quantum theory is assumed to be valid for all physical phenomena – at least as long as new experimental evidence will not teach us otherwise – but classical theories provide good approximations in many situations. Therefore it makes sense to try to develop an algebraic framework also for classical physics – not obvious as this may look at first sight. One of the advantages of such a general formulation is that it would narrow the conceptual gap between classical and quantum physics. In any case, a desire for unification has always been a guiding thought in theoretical physics.

Before I discuss in more detail my algebraic scheme for both classical and quantum physics, I shall remind you of some basic mathematical properties of algebras.

4.2. Reminder : Algebras

1. *Algebras*: An algebra $\mathcal{A}$ is a vector space with an additional multiplication

$$(a, b) \;\mapsto\; ab,$$

which is associative and distributive with respect to the vector space addition.

Note : A vector space can be real or complex, for us usually complex.

We shall make a general distinction between 'abstract' algebras, just 'abstract' vector spaces with an additional multiplication satisfying the above requirements, and 'concrete' algebras, algebras of functions (commutative) and algebras of matrices or linear transformations (in general noncommutative).

In these lectures we assume that associative algebras – so not Lie algebras – have a unit element.

2. $*$-*Algebras*: $\mathcal{A}$ is a $*$-algebra iff there is a conjugate linear map

$$a \mapsto a^*,$$

with the properties

$$(a^*)^* = a, \;\; (ab)^* = b^* a^*, \;\; (\lambda a)^* = \overline{\lambda} a^*, \quad \forall a, b \in \mathcal{A}, \;\; \lambda \in C^1.$$

A $*$-algebra is often called an *involutive algebra*, with the $*$-operation an *involution*. Anyway, do not confuse this notion with the *star product* of formal deformation quantization!

3. *Banach* $*$-*algebras*: A *normed algebra* has as a vector space norm, i.e. an assignment

$$a \mapsto ||a||,$$

with

$$||a|| \geq 0, \;\; ||a|| = 0 \;\Leftrightarrow\; a = 0, \;\; ||\lambda a|| = |\lambda| ||a||, \;\; \forall a \in \mathcal{A}, \;\; \lambda \in C^1,$$

and

$$||a + b|| \leq ||a|| + ||b||, \;\; \forall a, b \in \mathcal{A}. \text{ (triangle inequality)}$$

As an algebra norm it has the additional property

$$||ab|| \leq ||a||\, ||b||, \;\; \forall a, b \in \mathcal{A} \quad \text{(submultiplicativity)}.$$

For a $*$-algebra one has moreover

$$||a^*|| = ||a||, \;\; \forall a, b \in \mathcal{A}.$$

A *Banach* $*$-*algebra* is a normed $*$-algebra which is complete in its norm (Cauchy sequences are convergent). Finally :

4. A C^*-*algebra* is a Banach $*$-algebra $\mathcal{A}$ with a norm which satisfies

$$||a^*a|| = ||a||^2, \quad \forall a \in \mathcal{A}.$$

This innocent looking additional requirement has important consequences; it makes $\mathcal{A}$ into a C^*-algebra, one of the most important, interesting, and most studied objects in functional analysis.

So far we have looked at algebras, in particular C^*-algebras, as 'abstract' objects. We next discuss two important representation theorems, both due to I.M. Gelfand and M. Naimark.

- a. *For commutative C^*-algebras*: An 'abstract' commutative C^*-algebra is isomorphic to the algebra $C(X)$ of all continuous functions on some compact topological space X. The norm of a function in $C(X)$ is its supremum; the $*$-operation (involution) is complex conjugation. This makes it into a C^*-algebra. The correspondence of 'abstract' commutative C^*-algebras with algebras $C(X)$ is one-to-one, up to isomorphisms.

- b. *For noncommutative C^*-algebras*: A noncommutative C^*-algebra is isomorphic to a subalgebra of $B(\mathcal{H})$, the algebra of all bounded operators in a Hilbert space $\mathcal{H}$. So there is a one-to-one correspondence between 'abstract' noncommutative C^*-algebras and C^*-algebras of Hilbert space operators, again up to isomorphisms.

5. *von Neumann algebras*:

Von Neumann algebras are not 'abstract' algebras, but algebras of bounded operators in a Hilbert space.

Two equivalent definitions:

A topological definition : A von Neumann algebra is a strongly closed $*$-subalgebra of the algebra of all bounded operators in a Hilbert space.

Any $*$-algebra $\mathcal{B}$ of operators in $\mathcal{H}$ can be closed in this strong operator theory. This closure will be a von Neumann algebra, the smallest von Neumann algebra containing $\mathcal{B}$, or the von Neumann algebra generated by $\mathcal{B}$. We shall see an important example of further on.

Intermezzo : Convergence in operator algebras

Bounded operators have a norm $||\cdot||$

$$||A|| = \sup_{||\psi||=1} ||A\psi||.$$

A sequence of operators $\{A_n\}_n$ converges *in norm* to an operator A iff

$$\lim_{n\leftarrow\infty} ||A - A_n|| = 0.$$

It converges em strongly iff

$$\lim_{n\leftarrow\infty} ||(A - A_n)\psi|| = 0, \quad \forall\psi \in \mathcal{A}.$$

Strong convergence is, surprisingly, weaker than norm convergence. In operator algebra theory many other topologies, implying other types of convergence are used. We do not need them here.

An algebraic definition of von Neumann algebras : The commutant of a $*$-subalgebra $\mathcal{A}$ of $B(\mathcal{H})$, the algebra of all bounded operators in a Hilbert space $\mathcal{H}$, is the collection of all bounded operators commuting with all operators in $\mathcal{A}$. This set, denoted as $\mathcal{A}'$, is again a $*$-subalgebra of $B(\mathcal{H})$. The algebra $\mathcal{A}$ is a von Neumann algebra iff $\mathcal{A} = (\mathcal{A}')'$, i.e. iff it is its own double commutant.

C^*-algebras versus von Neumann algebras

Von Neumann algebras contain all the projection operators of their selfadjoint elements (Important for quantum theory). C^*-algebras do not.

Example: The algebra of all continuous functions on $[0, 1]$ is a commutative C^*-algebra; it contains no projections at all; the larger algebra of all bounded measurable functions on $[0, 1]$ has many projections.

Note that $B(\mathcal{H})$ is both a C^*-algebra and a von Neumann algebra.

This should be sufficient for our purpose about the general properties of various types of algebras. For more details, see ("Algebras, States and Representations". See also Refs [1]-[11] for much more details.

4.3. A general algebraic framework

After this preliminary mathematical material we return to the discussion of what is the main subject of this lecture, an algebraic

framework, in which classical physics is obtained as a special case by requiring the relevant algebras to be *commutative*, and in turn quantum physics appears as a generalization – or perhaps a deformation – of classical physics.

It is true that this does not add much, concretely and explicitly, to known theories, except in the case of systems with an infinite number of degrees of freedom, thermodynamic limit for classical and quantum statistical mechanics and relativistic quantum field theory. It is not helpful in performing calculations. It also has loose ends. Considerable white areas remain; many details have not been worked out, but all this does not diminish its conceptual attraction.

The general idea of this approach may be illustrated by a recent mathematical development that connects algebra and geometry in a new way, a development which may be seen as a background for our general scheme.

It is called *"noncommutative geometry"*, has as its origin the work of Gelfand and Naimark on the one-to-one correspondence between compact topological spaces and commutative C^*-algebras and has been developed into a broad mathematical discipline by the French mathematician Alain Connes. See for this his book (Ref.[12]) and also the book of Gracia-Bondia et al (Ref.[13]). The general idea of this is – very naively formulated, first the observation that many mathematical theories start from a 'space', i.e. a point set with additional structure, for instance a measure space, a topological space or a differentiable manifold, and secondly that such a 'space' can be characterized by a *commutative algebra*, namely the algebra of the appropriate functions on the underlying set, measurable, continuous and smooth functions.

The next step, the truly interesting one, is then that by looking at similar *noncommuting algebras* new mathematical theories are obtained based on 'virtual spaces', which have no meaning as point sets, but are intuitive ideas that suggest interesting generalizations of properties of the commutative case.

In this spirit the general theme of this lecture will be:

Classical physics $\longleftrightarrow$ **Commutative algebras**
Quantum physics $\longleftrightarrow$ **Noncommutative algebras**

In this scheme the algebras are of the same type, e.g. commutative and noncommutative C^*-algebras, or commutative and noncommutative von Neumann algebras, etc., notions that we have just briefly described.

As I stated at the beginning of this lecture, ideas of this type have been around already for some time and are discussed at various places in the literature; see for instance the recen books by Faddeev and Yakubovskiĭ, an excellent short introduction, however with not much details (Ref.[14]). There is also the book of Strocchi (Ref.[15], p.10-23). The approach in this book is however mathematically too narrow. The purpose of this lecture to develope this ideas in a more systematic way.

A proposal of formulating quantum physics in terms of abstract algebras of observables with averages given by positive linear functionals on these algebras was first put forward in 1947 by I. E. Segal in a classic paper (Ref.[16]) and applied later by others to specific topics in quantum physics, in particular to attempts to give a rigorous mathematical basis to quantum systems with an infinite number of degrees of freedom such as quantum field theory and quantum statistical mechanics in the thermodynamic limit. See the seminal paper by Haag and Kastler (Ref.[17]). However, the mathematical basis was laid earlier by the work of Gelfand and Naimark, with as central point their representation theorem for commuting C^*-algebras (Ref.[18]).

4.4. Spaces / 'Spaces'. Commutative / Noncommutative

4.4.1. Introduction

The central idea of this lecture is that of 'space'. First as a precise notion: a point set X, carrying an additional structure characterized by the commutative algebra $C(X)$ of appropriate functions on X, which characterizes this structure. Then, in a more suggestive and heuristic way, in the quantum situation, there is no longer a point set X, but there is the noncommutative version of the algebra $C(X)$ from the classical case, no longer an algebra of functions but still suggesting in a heuristic way an underlying 'space'.

4.4.2. A list of spaces and their associated 'spaces'

In this subsection we present an annotated list of 'spaces' and their virtual noncommutative analogues. For more mathematical details see the supplementary text "Algebras, states and representations".

(1) *Topological spaces.*

The history of the subject begins with the theorem of Gelfand and Naimark, which states that there is a one-to-one correspondence between commutative C^*-algebras and compact topological spaces. See "Algebras, states and representations, Section 4".

This leads to a suggestion for noncommutative C^*-algebras :

'compact quantum topological space' means *"noncommutative C^*-algebra".*

(2) *Measure spaces* or *probability spaces.*

(Measure spaces /probability spaces) There is a similar relation between commutative von Neumann algebras and algebras of measurable functions on measure spaces or, more in particular, a probabilty space, which is a bit more complicated because it is a correspondence between equivalence classes. More details in ("Algebras, states and representations. Section 5").

This leads to a suggestion for noncommutative von Neumann algebras :

'quantum measure' or *'probability space'* means *"noncommutative von Neumann algebra".*

(3) *Smooth manifolds*

Smooth, or differentiable, manifolds are topological manifolds with a differentiable structure (See "Manifolds"). The associated algebra of smooth functions $C^\infty(\mathcal{M})$ has for a compact manifold $\mathcal{M}$ a Fréchet spac as its underlying vector space, and for a noncompact $\mathcal{M}$ a LF space, i.e. a direct limit of a sequence of Fréchet spaces.

Reminder: *Fréchet spaces and algebras*. A *locally convex space* is a topological vector space with a topology determined by a *single* norm $||\cdot||$, but by a system $\{||\cdot||_\alpha\}_{\alpha\in\mathcal{I}}$. of *seminorms.* A norm has the same properties as a norm except that $||a||_\alpha = 0$ does not imply $a = 0$. A *Fréchet space* is a complete locally convex space, with a topology determined by a countable set of semi norms and that is

moreover *metrizable*. For a *Fréchet algebra* $\mathcal{A}$ the seminorms have to satisfy the submultiplicativity property

$$||ab||_\alpha \leq ||a||_\alpha \, ||b||_\alpha, \quad \forall \alpha \in \mathcal{I}, \quad a, b \in \mathcal{A}.$$

No full analogue of the Gelfand-Naimark theorem for commutative C^*-algebras is known for the algebras of smooth functions on manifolds. There is however the following remarkable theorem (Thomas. Ref.[19]):

Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be two manifolds, with their algebras of smooth functions $C^\infty(\mathcal{M}_1)$ and $C^\infty(\mathcal{M}_2)$. Suppose that the function algebras $C^\infty(\mathcal{M}_1)$ and $C^\infty(\mathcal{M}_2)$ are isomorphic. Then $\mathcal{M}_1$ and $\mathcal{M}_2$ are diffeomorphic.

This leads to an admittedly rather vague suggestion for noncommutative smooth $*$-algebras :

'quantum manifold' means *"noncommutative smooth $*$-algebra"*.

Note that if we restrict to bounded smooth functions, the corresponding noncommutative smooth $*$-algebra will be a subalgebra of a C^*-algebra.

(4) *Symplectic manifolds*

A symplectic manifold is a smooth manifold provided with a symplectic form, i.e. a closed nondegenerate 2-form ω, which defines a *Poisson bracket* $\{\cdot, \cdot\}$ on the algebra of smooth functions $C^\infty(\mathcal{M})$ according to $\{\cdot, \cdot\}$ on $C^\infty(\mathcal{M})$:

$$\{f, g\} = \omega(X_f, X_g), \quad \forall f, g \in C^\infty(\mathcal{M}).$$

and with X_f, X_g the Hamiltonian vector fields associated with f, g.

Remember that a vector field X_h is called Hamiltonian, associated with the function h, iff

$$dh(Y) = \omega(X_h, Y), \quad \text{for all vector fields } Y.$$

The Poisson bracket makes $C^\infty(\mathcal{M})$ into a *Poisson algebra*.

A manifold with a Poisson bracket is called a *Poisson manifold*, and is slightly more general than a symplectic manifold. Poisson geometry, as a special topic in differential geometry, has been thoroughly investigated. Less attention has been paid to the functional

analytic properties of $C^\infty(\mathcal{M})$, as a special case of a locally convex topological algebra.

This nevertheless leads to a suggestion for noncommutative Poisson $*$-algebras:

'Quantum Poisson manifold' means *"noncommutative smooth Poisson $*$-algebra"*.

There is a one-to-one correspondence between the algebras of continuous functions on compact topological spaces and commutative C^*-algebras, so an arbitrary noncommutaive C^*-algebra can be thought of as representing a *'noncommutative compact topological space'*. There is also a one-to-one correspondence between the algebras of (essentially) bounded measurable functions on measure spaces and commutative von Neumann algebras, so a noncommutative von Neumann algebra can be thought of as representing a *'noncommutative measure space'*. Unfortunately, for the cases of smooth quantum manifolds and even more for quantum Poisson manifolds, one has only suggestions. The smooth functions on manifolds are Fréchet or LF algebras, characterizing the manifolds, as the theorem of Thomas tells us, but we do not know what particular type of these algebras describe in this manner smooth manifolds. For Poisson manifolds we know even less.

Two rather different areas of mathematics, using different concepts, are relevant for quantum theory:

1. *Functional analysis*: Provides the language for quantum theory as mathematically formulated by von Neumann. This is expressed in the axiom systems 'Version 1' and 'Version 2', discussed in the preceding lectures. For all practical physical purposes this approach is satisfactory; it provides everything one needs.

2. *Symplectic differential geometry* or a bit more general *Poisson geometry*: One important aspect of both classical and quantum mechanics is missing from von Neumann's axiom system, its Hamiltonian structure. This is basic and clearly present in classical mechanics, with a general phase space in a natural manner a symplectic manifold and time evolution and all symmetries canonical transformations leaving this structure invariant. It is of importance when studying quantum mechanics as deformation of classical mechanics, with Planck's constant $\hbar$ as a the deformation parameter. This will

be taken up in the next lecture. Here, in the context of setting up our 'Version 3' of an axiom system for quantum theory, we shall only discuss a function analytic approach. The main topic of this school is Poisson geometry, so you will hear more about symplectic aspects in some of the other lectures.

4.5. The third version of our axiom system

4.5.1. Introduction

In our first lecture we formulated 'Version 1' of our system of axioms for quantum theory, with as basic notions unit vectors in a Hilbert space as states and selfadjoint operators in that space as observables. A second level of axiomatics, 'Version 2', was introduced in the third lecture, still with a Hilbert space, but this no longer as the space of states, but as an ambient background space, and now the states being described by density operators. This generalization was necessary for the description of quantum statistical physics. The use of these two levels is standard in mainstream quantum physics.

In this section we are going to introduce 'Version 3'. It is an axiom system, in which one starts from an abstract algebra, much in the spirit of Refs.[16],[17],[20],[21],[22]. This third formalism is not – or, maybe, not yet – part of the standard curriculum of physics. It is of great conceptual interest as a general theoretical framework, but has in a practical sense not much to offer in ordinary classical and quantum mechanics. It does however play an important role in the description of systems with an infinite number of degrees of freedom, the thermodynamic limit in statistical physics, both classical and quantum, and relativistic quantum field theory.

4.5.2. A sketch of 'Version 3'

We first give a rough version of the third axiom system, and after that a more precise and detailed one for two specific situations.

Observables

- Axiom I$''$: Observables : *a complex $*$-algebra $\mathcal{A}$.*

States

- Axiom II$''$: States : *positive normalized linear functionals ω on $\mathcal{A}$.*

A state on a $*$-algebra $\mathcal{A}$ is a positive normalized linear functional on $\mathcal{A}$. This definition comes from physics but is now generally used by mathematicians.

Physical interpretation:

- Axiom III$''$: Axiom I$''$ and Axiom II$''$ are combined to give probabilistic predictions for measurements, along the same lines as earlier in 'Version 1' and 'Version 2'.

Time evolution / Symmetries

In some situations either time evolution does not play a role (statistical mechanics, or is absorbed in symmetry. This will be explained when discussing the more detailed version of this axiom system.

- Axiom IV$''$: Time evolution : *a 1-parameter group $\{\phi(t)\}_{t\in R^1}$, of $*$-automorphisms of $\mathcal{A}$.*

- Axiom V$''$: *Symmetries :* various $*$-automorphisms and groups of $*$-automorphisms of $\mathcal{A}$, commuting with the time evolution automorphisms.

4.5.3. Axiom system 'Version 3' for two specific situations

Although on this third level the starting point is not a Hilbert space, but the *algebra of observables*, a state dependent Hilbert space will nevertheless automatically emerge from the data specified according to the first two axioms. This will be explained further on. Here follows the list of axioms again, now in more detail and for specific situations.

4.5.4. Observables

- Axiom I$''$: *There is an abstract C^*-algebra $\mathcal{A}$ of what I call* pre-observables*, the 'skeleton' of a von Neumann operator algebra of* physical observables,

This von Neumann algebra will emerge naturally in the setting up of a system in Version 3.

Note: When a C^*-algebra $\mathcal{A}$ is represented as an operator algebra in a Hilbert space by a representation π, the projections of its self-adjoint elements do not necessarily belong to the algebra, nor to its image $\pi(\mathcal{A})$. They do however belong to the closure of $\pi(\mathcal{A})$ in the strong operator topology. This closure is a von Neumann algebra, the von Neumann algebra generated by $\mathcal{A}$, which I shall denote as

$\widehat{\mathcal{A}}$. It is the physically relevant object. It is important to realize that this a representation dependent object. I could have denoted it as $\widehat{\mathcal{A}}_\pi$.

A physical system is characterized by its algebra of observables. For 'Version 3' of the axiom system for quantum theory, as we present it here, is meant for two types of systems, both with an infinite number of degrees of freedom.

1. *Statistical mechanics in the thermodynamic limit*, i.e. in the limit where the number of finite subsystems goes to infinity. One considers a partially ordered system of finite subsystems of increasing size, e.g. a system of d-dimensional spatial lattices $\{\Lambda_\alpha\}_{\alpha\in\mathcal{I}}$, with elementary magnets at each sites, interacting with each other. The variables of each subsystem form a finite dimensional C^*-algebra $\mathcal{A}_\alpha$ – every finite dimensional $*$-algebra is of course a C^*-algebra. These algebras form an inductive system. This means, without giving a precise definition, that an algebra of a smaller subsystem can be injected in a natural manner into the algebras of a larger system, leading to a single all-encompassing C^*-algebra of 'quasilocal' observables which is the algebra $\mathcal{A}$ of Axiom I$''$. By considering states on this algebra – see Axiom III$''$, one hopes to be able to describe aspects of the coexistence of more than one phase, separated by a phase transition. In both classical and quantum statistical mechanics one is mainly interested in *equilibrium states*, which means that there is no time evolution, so in this case there is no need for Axiom VI$''$. Symmetries, Axiom V$''$, in particlar spatial rotations and translations, remain important. See for the subject of the rigorous mathematical treatment of the thermodynamic limit in statistical mechanics Refs.[20], [21].

2. *Relativistic quantum field theory.* This topic will be discussed in Lecture 6. However, it is useful to discuss in the context of this lecture the characterization of its algebra of observables, in the algebraic approach of Araki, Haag and Kastler. See Ref.[17].

In this approach there are no field operators, but local C^*-algebras attached to open sets of spacetime, a 4-dimensional affine space, the theatre of the special theory of relativity. All this will be discussed in more detail in Lecture 6. This means that there is a inductive system $\{\mathcal{A}_O\}_{O\subset R^4}$ of local C^*-algebras, which give one all-encompassing C^*-algebra of *quasi-local observables* $\mathcal{A}$. There is no notion of a separate

time evolution, which means that Axiom VI″ (time evolution) is absorbed by Axiom V″ (symmetry)

4.5.5. States

- Axiom II″: *There is a convex set of* states*, the collection* $\mathcal{S}$ *of positive normalized linear functionals on* $\mathcal{A}$.

The name 'state' for such a functional comes from physics; it is now in general use by mathematicians, in particular mathematicians working in operator algebras. A state ω determines a representation π_ω of $\mathcal{A}$ in a Hilbert space $\mathcal{H}_\omega$, the so-called *GNS-representation*. The strong closure of π_ω of $\mathcal{A}$, the operator algebra $\widehat{\mathcal{A}}_\omega$, is the representation dependent von Neumann algebra of physical observables.

The GNS–representation – GNS = Gelfand-Segal Naimark, is the central mathematical object of this system of axioms. I shall sketch its construction. It is one of these typical constructions that mathematicians love; one starts with a mathematical object, a group, an algebra, then by letting it act on it self one gets interesting results.

4.5.6. An intermezzo: The GNS construction

Let $\mathcal{A}$ be a given C^*-algebra, and ω a given state. To obtain our representation we let $\mathcal{A}$ act on it self. One has to realize that in this procedure $\mathcal{A}$ plays two roles, as the algebra that is represented and as the representation space. We define the first stage of the representation as

$$\pi_0(a)b = ab, \ \ \forall a, b \in \mathcal{A}.$$

One verifies easily that this defines a representation of $\mathcal{A}$ into linear operators in $\mathcal{A}$ itself. The state ω defines a sesquilinear form on $\mathcal{A}$ according to

$$(a, b)_0 = \omega(a^*, b), \quad \forall a, b \in \mathcal{A}.$$

This form is degenerate, it is almost an inner product, positive but with null-vectors. These can be removed by going to a quotient space. Define $\mathcal{I}$ in $\mathcal{A}$ as

$$\mathcal{I} =: \{a \in \mathcal{A} \mid (a, a)_0 = \omega(a^*a)\} = 0.$$

This is a *left ideal* in the algebra $\mathcal{A}$, i.e. a linear subspace $\mathcal{I}$ with the property

$$a \in \mathcal{I} \iff ab \in \mathcal{I}, \ \ \forall b \in \mathcal{A}.$$

Although $(\cdot,\cdot)_0$ is not strictly positive definite, the Schwarz inequality holds.

Problem: Use this to prove that $\mathcal{I}$ is indeed a left ideal.

Answer: Let a be in $\mathcal{I}$ and b in $\mathcal{A}$.

$$(ba, ba)_0 = \omega((ba)^* ba) = \omega(a^* b^* ba) = (a, b^* ba)_0,$$

so

$$|(ba, ba)_0| = |(a, b^* ba)_0| \leq |(a, a)_0|^{1/2} |(b^* ba, b^* ba)_0|^{1/2} = 0,$$

which proves that ba an element of $\mathcal{I}$ is, for all a in $\mathcal{A}$, i.e. $\mathcal{I}$ is a left ideal in $\mathcal{I}$.

With this ideal we define an equivalent relation in $\mathcal{A}$ by

$$a \sim b \iff a - b \in \mathcal{I}.$$

This equivalence relation gives a quotient space $(\mathcal{H}_\omega)_0 = \mathcal{A}/\sim$, a pre-Hilbert space that can be completed in the usual manner to a Hilbert space $\mathcal{H}_\omega$. Due to the fact that $\mathcal{I}$ is a left ideal, the operators $\pi(a)$ descend to operators $\pi_\omega(a)$ on $(\mathcal{H}_\omega)_0$ and can then be extended to bounded operators in $\mathcal{H}_\omega$. This is the GNS-representations, associated with the state ω. So we have a Hilbertspace $\mathcal{H}_\omega$, with the GNS representation π_ω of the algebra $\mathcal{A}$ of pre-observables. The representing algebra $\pi_\omega(\mathcal{A})$ generates a von Neumann algebra by taking the strong closure of $\pi_\omega(\mathcal{A})$. This closure is the representation dependent algebra of observables.

There is a special vector in $\mathcal{H}_\omega$, n.l. $\psi_0 = [1]$, the equivalence class containing the unit element of $\mathcal{A}$. Every vector ψ in $(\mathcal{H}_\omega)_0$ is an equivalence class $[a]_\sim$ for some a in $\mathcal{A}$. This means that every ψ can be written as $\psi = \pi_\omega(a)\psi_0$, for some a in $\mathcal{A}$. These vectors are dense in $\mathcal{H}_\omega$ because, by definition, $(\mathcal{H}_\omega)_0$ is dense in $(\mathcal{H}_\omega)$, One says that ψ_0 is a *cyclic vector for the representation* π_ω. An important theorem that I shall not prove states that π_ω is irreducible if and only if ω is pure.

4.5.7. Physical interpretation

Axiom III$''$: *The physical interpretation in terms of the results of the measurement of an observable A in a state ω combines Axioms*

I″ and II″ and follows the same line as in the two earlier versions of the axiom system.

We have again a Hilbert space, the GNS-representation space $\mathcal{H}_\omega$. In general this is not the Hilbert space of states from 'Version 1', nor the background Hilbert space from 'Version 2'. The algebra $\mathcal{A}$ is represented by a C^*-algebra of bounded operators $\pi_\omega(\mathcal{A})$. The algebra of bounded physical observables is the closure in the strong topology of this, the von Neumann algebra $[\pi_\omega(\mathcal{A})]''$. It contains all the projection operators belonging to the selfadjoint operators in $\pi_\omega(\mathcal{A})$.

For ω pure the representation π_ω is irreducible. Schur's lemma tells us that this implies that the commutant of $\pi_\omega(\mathcal{A})$ consist of only the multiples of the unit operator, and that therefore its double commutant is the algebra $B(\mathcal{A})$ of all bounded operators in $\mathcal{H}_\omega$. So the von Neumann algebra of physical operators is $B(\mathcal{A})$. This implies that in this case we are back in the situation of 'Version 1': $\mathcal{H}_\omega$ is the Hilbert space of state vectors; de state ω is represented by the state vector ψ_0.

A mixed state ω may be representable by a density matrix, with $\mathcal{H}_\omega$ as background Hilbert space. In that case we are back in 'Version 2'. For a system with an infinite number of degrees of freedom this will not happen; 'Version 3' is than an essential generalization.

4.5.8. Time evolution / Symmetries

Axiom IV″: *The time evolution of a system is described by a* 1*-parameter groups of* $*$*-automorphisms* $\{\phi_t\}_{t\in R^1}$ *of* $\mathcal{A}$ *acting on the state* ω *as*

$$\omega_{\phi_t}(A) = \omega(\phi_{-t}(A))\,, \qquad \forall A \in \mathcal{A}\,.$$

Time evolution automorphisms should be unitarily implementable in $\mathcal{H}_\omega$, i.e. there should exist 1-parameter groups of unitary operators U_{ϕ_t} acting in the GNS-representation Hilbert space $\mathcal{H}_\omega$, such that

$$\pi_\omega(\phi_t(A)) = U_t^{-1}\pi_\omega(A)\,U_t, \quad \forall t \in R^1,\, A \in \mathcal{A}.$$

A state ω on $\mathcal{A}$ is called *invariant* with respect to the time evolution automorphisms iff

$$\omega_0(A) = \omega_0(\phi_{-t}(A))\,, \qquad \forall A \in \mathcal{A}\,, \qquad \forall t \in R^1\,.$$

Invariance of ω implies unitary implementability. It is convenient to requires continuity for the 1-parameter group $\{\phi_t\}_{t\in R^1}$, such that there is strong continuity for the group $\{U_t\}_{t\in R^1}$.

Axiom V″: *Symmetries, (groups of symmetries) of physical systems are described by $*$-automorphisms (groups of $*$-automorphisms) of $\mathcal{A}$, that commute with the time evolution automorphisms.*

Symmetry automorphisms are always required to leave the state ω invariant, are therefore unitarily implemented by a unitary operators in the GNS-representation space $\mathcal{H}_\omega$, and consequently leaves the state vector ψ_0 invariant.

For the sake of generality I have given here both axioms Axiom IV″ and V″, even though we have no time evolution in equilibrium states in statistical mechanics, and even though time evolution is absorbed in the notion of symmetry in relativistic quantum field theory.

Note that the statistical mechanical models in this situation may be classical or quantum; for the field theory only the quantum case makes in this context sense.

This completes our description 'Version 3' of our axiom system, applied to two situations, the thermodynamic limit in statistical mechanics and relativistic quantum field theory in the algebraic approach.

4.6. Appendix. An algebraic form of differential geometry

4.6.1. Introduction

In this appendix I shall discuss an algebraic approach to differential geometry in which one derives all properties of and structures on a manifold $\mathcal{M}$ from the derivations of the algebra $C^\infty(\mathcal{M})$ of smooth functions, in such a way that the points of the manifold play no role. This approach is due to J.L. Koszul (Ref.[23]).

4.6.2. $\mathcal{A}$-linear algebra

Let $\mathcal{A}$ be a commutative real algebra, associative and with unit element. At the end of this note I shall take for $\mathcal{A}$ the algebra $C^\infty(\mathcal{M})$ of smooth functions on a manifold $\mathcal{M}$.

Definition: An *$\mathcal{A}$-module* is a real vector space V which has in addition to multiplication by real numbers a multiplication by elements

from $\mathcal{A}$

$$(a, x) \ \mapsto ax, \ \forall a \in \mathcal{A}, \ x \in V.$$

This multiplication satisfies the usual properties of associativity, and distributivity with the addition.

The properties of a module over a commutative algebra are very much the same as those of a vector space. One can perform all the usual operations of ordinary linear algebra.

Let V_1 and V_2 be two $\mathcal{A}$-modules. A map $T : V_1 \to V_2$ is called $\mathcal{A}$-*linear* if it is linear over de real numbers and if one has moreover

$$T(ax) = aT(x), \ \forall a \in \mathcal{A}, \ x \in V_1.$$

An $\mathcal{A}$-module V has a dual V^*, the $\mathcal{A}$-module of all $\mathcal{A}$-linear maps $F : V \to \mathcal{A}$. The definition of a $\mathcal{A}$-tensor product of $\mathcal{A}$-modules $(V_1, V_2, \ldots, V_N)$,

$$V_1 \otimes_{\mathcal{A}} V_2 \otimes_{\mathcal{A}} \ldots \otimes_{\mathcal{A}} V_n$$

is analogous to the definition for vector spaces, as is the definition of symmetric and antisymmetric $\mathcal{A}$-tensor products.

4.6.3. Derivations

Let $\mathcal{A}$ be as before. A *derivation* of $\mathcal{A}$ is a linear map $D : \mathcal{A} \to \mathcal{A}$, with the *Leibniz* property

$$D(ab) = D(a)b + aD(b), \ \forall a, b \in \mathcal{A}.$$

The derivations form an $\mathcal{A}$-module. They form moreover a Lie algebra. Both properties can be checked easily. We denote the $\mathcal{A}$-module of derivations as $V_1(\mathcal{A})$.

4.6.4. Differential geometry

Consider finally a manifold $\mathcal{M}$, with $\mathcal{A} = C^\infty(\mathcal{M})$ the (commutative, associative) algebra of its smooth functions.

Theorem: A (smooth) vector field on $\mathcal{M}$ is a derivation of $C^\infty(\mathcal{M})$ and each derivation of $C^\infty(\mathcal{M})$ is a (smooth) vector field on $\mathcal{M}$.

The first part of the theorem is fairly obvious; the proof of second part is nontrivial. It can be found in any good textbook on differential geometry. This part of the theorem is central for our approach

to differential geometry. Note that it means that one does not need any assumption about continuity or smoothness, in what ever sense. One obtains smooth vector fields in a purely algebraic manner.

We have an 'almost' Gelfand-Naimark theorem for manifolds. A theorem by Thomas states that two manifolds that have isomorphic algebras of smooth functions are diffeomorphic.

It means that a manifold $\mathcal{M}$ is completely determined by its commutative algebra $\mathcal{A} = C^\infty(\mathcal{M})$. In fact the manifold can be reconstructed from $C^\infty(\mathcal{M})$ as an 'abstract' algebra. From this algebra we obtain the module of its derivations and then use linear algebra in the sense of $C^\infty(\mathcal{M})$-modules to derive from this module all objects and structures on $\mathcal{M}$ without ever looking at $\mathcal{M}$ or its points again.

We have in the first place the vector fields on $\mathcal{M}$ as the $C^\infty(\mathcal{M})$-module $V_1(C^\infty(\mathcal{M}))$. From this we obtain the module of 1-forms as its dual, and by taking antisymmetric tensor products of this the modules of general p forms $\Omega_p(C^\infty(\mathcal{M}))$. The exterior derivative d, which, as one find in books, has a completely algebraic definition in term of the basic module of vector fields, is therefore defined here in a similar way by explicit use of $C^\infty(\mathcal{M})$-module linear algebra.

By taking all possible tensor products from the $C^\infty(\mathcal{M})$-module of derivations of $C^\infty(\mathcal{M})$ and its $C^\infty(\mathcal{M})$-dual one obtains all possible contravariant, covariant and mixed tensor fields on $\mathcal{M}$.

All this is linear algebra in the sense of $C^\infty(\mathcal{M})$-module, beginning with the derivations of the algebra $C^\infty(\mathcal{M})$.

Poisson brackets, Riemannian metrics, connections, vector bundles with their sections, all arise in a purely algebraic way from the algebra $C^\infty(\mathcal{M})$ as an 'abstract' algebra and subsequently the from the 'abstract' $C^\infty(\mathcal{M})$-module of derivations of this algebra by linear algebra in the sense of $C^\infty(\mathcal{M})$-modules.

4.7. References

• *References on algebras, in partcular C^*-algebras, von Neumann algebras, operator algebras*

[1]. J. Dixmier
C-algebras*

Translated from the 1969 French edition
North-Holland / Elsevier 1977

[2]. J. Dixmier
Von Neumann Algebras
Translated from the second French edition 1969
(First French edition 1957)
North-Holland 1981

Important basic books, although by now somewhat outdated, in particular the second book, because of the emergence of the so-called 'modular theory' after its publication. Written in typical Bourbaki style; clear, precise, dry.

The French edition of both books are still available, certainly second hand.

[3]. Gerard J. Murphy
C^*-Algebras and Operator Theory
Academic Press 1990

[4]. William Arveson
An Invitation to C^*-Algebras
Springer 1976. Corrected second printing 1998

[5]. Ola Bratteli, Derek W. Robinson
Operator Algebras and Quantum Statistical Mechanics II. Equilibrium States. Models in Quantum Statistical Mechanics
Springer 1981

[6]. John B. Conway
A Course in Operator Theory
American Mathematical Society 2009

[7]. Jacob T. Schwartz
W^*-Algebras
Gordon and Breach 1967

Note that W^*-algebra is a rather old-fashioned name for von Neumann algebras.

[8]. Vaughan F.R. Jones
Von Neumann Algebras
Lecture Notes 2010

Available at :
`http://www.math.berkeley.edu/~vfr/MATH20909/VonNeumann2009.pdf`

Six useful, readable introductions. (Part I of [5]).

[9]. Bruce Blackadar
Operator Algebras. Theory of C^*-Algebras and von Neumann Algebras
Springer 2006

[10]. Richard V. Kadison, John R. Ringrose
Fundamentals of the Theory of Operator Algebras
Volume I: Elementary Theory
American Mathematical Society 1997

[11]. Masamichi Takesaki
Theory of Operator Algebras I
Springer 1979. Second printing 2001

The first volumes of these two series are solid books of reference on operator algebra theory.

Three more comprehensive textbooks.

[12]. Alain Connes
Noncommutative Geometry
Academic Press 1994

Available at his website :
`http://www.alainconnes.org/docs/book94bigpdf.pdf`

One of the great mathematics books written in the last twenty years. "The reader of the book should not expect proofs of theorems. This is much more a tapestry of beautiful mathematics and physics which contains material to intrigue readers ..." (Vaughan Jones). "... a long discourse or letter to friends" (I.E. Segal in a review - Bull.Amer. Math. Soc. 33, 459-465 (1996). The author was not amused). The serious student will get much help from the next book:

[13]. José M. Gracia-Bondía, Joseph C. Varilly. Hector Figueroa
Elements of Noncommutative Geometry
Birkhauser 2001

The best general textbook on noncommutative geometry in the spirit of Connes. The 'authorized version' at the time this book was published.

[14]. L.D. Faddeev, O.A. Yakubovskii
Lectures on Quantum Mechanics for Mathematics Students
Translated from the Russian
American Mathematical Society 2009

Written in a clear and engaging style, with a perfect balance between physics and mathematics, and emphasizing an algebraic point of view that unifies classical and quantum mechanics. It is however too short to provide much mathematical det

[15]. F. Strocchi
An Introduction to the Mathematical Structure of Quantum Mechanics
World Scientific 2005

A short series of lectures, containing many interesting details. Classical and quantum mechanics are seen as different realizations of the same algebraic formalism as in [3], but the mathematical framework that the author employs for this is too narrow.

[16]. Irving E. Segal
Postulates for general quantum mechanics
Ann. Math. 48, 930-948 (1947)

The founding paper on the subject of this chapter.

[17]. Rudolf Haag, Daniel Kastler
An algebraic approach to quantum field theory
J.Math.Phys. 5, 848-861 (1964).

An important paper applying the ideas of [16] to quantum field theory.

[18]. I. M. Gelfand, M. A. Naimark
On the imbedding of normed rings into the ring of operators on a Hilbert space
Math. Sbornik 12, (197217) 1943

[19]. E.G.F. Thomas
Characterization of a manifold by the $*$-algebra of its C^∞ functions
Preprint Mathematical Institute, University of Groningen $\pm$ 1990
Unpublished.

Erik Thomas died on September 13, 2011. A little known but remarkable theorem, which uses standard functional analysis. Copies of this note can be obtained by sending me an e-mail.

[20]. David Ruelle
Statistical Mechanics. Rigorous Results. Second Edition
World Scientific 1999. First edition Benjamin 1969

[21]. David Ruelle
Thermodynamic Formalism. Second Edition
Cambridge University Press 2004, First edition Addison Wesley 1978

These two books discuss the formalism for the description of systems with an infinite number of degrees of freedom, in particular such as in classical and quantum statistical mechanics.

[22]. Huzihuro Araki
Mathematical Theory of Quantum Fields
Oxford University Press 2009

This book gives an introduction to the axiom system for algebraic quantum field theory, an example of what we call a 'Version 3' axiom system.

[23]. J.L. Koszul
Lectures on Fibre Bundles and Differential Geometry
Tata Institute of Fundamental Research. Bombay 1960.

Accessible at:
`http://www.math.tifr.res.in/~publ/ln/tifr20.pdf`

5. Quantization

5.1. Introduction

In this lecture I shall discuss 'quantization', a word with various slightly different meanings. The first meaning is historic. The founders of quamtum mechanics struggled with serious fundamental problem in physics – classical physics, we would say now. Heisenberg discovered that by employing noncommuting canonical variables he could correctly calculate the energy levels of the hydrogen atom. Schrödinger, inspired by the ideas of de Broglie about waves that accompany each particle, invented his wave equation.

This procedure of constructing quantum theories from known classical theories by 'quantizing' them, went on for several years. For example, Maxwell's theory was and is still a very good classical theory. A quantized version was constructed, at an early stage by Dirac, with important improvements later by Feynman and others in the nineteen forties. Then, with the discovery of new elementary particles, new quantum theories were formulated, for which there was no classical example. The π_0-meson was such a particle. It could be described by the Klein-Gordon quantum field, a system of so-called field operators satisfying a partial differential equation. There exist a numerical 'classical' Klein-Gordon equation, without any physical physical meaning. The same for the Dirac quantum field describing electrons and positrons. (We shall give an introduction to quantum field theory in the last lecture).

This last method has become standard: inventing a 'classical' equation, and then using this to find a physically meaningful quantization of this auxiliary non-physical theory. For boson systems the underlying classical or pseudo-classical has a Hamiltonian structure, involving a symplectic manifold, infinite dimensional in the case of fields. For fermion systems one needs an interesting generalization of symplectic geometry, *supersymplectic geometry* based on the notion of *supermanifold*. There will be no opportunity to discuss this in these lectures.

There is one quantization method in which a classical model is essential: *Feynman's path integral quantization*. It is a intuitive very attractive but heuristic procedure which leads from a classical model,

again possible fictitious, to quantum theoretical results such as transition amplitudes, without ever mentioning a Hilbert space of states. It uses measures and integrals over spaces of classical 'histories', which up till now have not been given a rigorous mathemathical meaning. This quantization method is very popular among elementary particle physicists, for generating diagrammatic terms in the perturbation series (*Feynman diagrams*), that they use to calculate the outcome of scattering experiments at very high energies. Again, there is no room to discuss this in these lectures.

In the end one should realize that quantum theory is the basic general theory describing all of the physical world – at least so we believe, as long as we are not contradicted by new experiments. It has to be used for submicroscopic phenomena, at the level of atoms and molecules, For most macroscopic situations, where we use units in which Planck's constant $\hbar$ is small, we may derive classical physics as a useful and precise *approximation*.

5.2. What is quantization?

Quantization, whatever its merits as a fundamental physical notion, is a procedure in which one assigns in a systematic way to a given classical physical system a quantum system, whether or not this a 'real' physical system or an auxiliary fictitious system. Let us start with a classical mechanical system with as phase space the symplectic manifold $\mathcal{M}$, here just R^{2n} with the standard symplectic form

$$\omega = \sum_{j=1}^{n} dp^j \wedge dq^j.$$

with its algebra $C^\infty(R^{2n})$ of smooth functions, which we complexify to a complex $*$-algebra $C_C^\infty(R^{2n})$ with $f \mapsto \overline{f}$ as the $*$-operator. We have the *Poisson bracket* between two functions from $C^\infty(R^{2n})$ as

$$\{f, g\} = \sum_{j=1}^{n} \left(\frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} - \frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} \right),$$

which makes $C^\infty(R^{2n})$ into a $*$-*Poisson algebra*. Note that the Poisson bracket is real, i.e. $\overline{\{f, g\}} = \{\overline{f}, \overline{g}\}$.

Definition: A quantization a classical system is a linear map $\mathcal{Q}$ from the functions f in $C_C^\infty(R^{2n})$ into operators $\mathcal{Q}(f)$ in $\mathcal{H}$, with

the property (1)

$$\mathcal{Q}(1) = 1_{\mathcal{H}},$$

and the reality condition (2)

$$\mathcal{Q}(\,\overline{f}\,) = \mathcal{Q}(f))^*.$$

There is a suggestive relation between the Poisson bracket for classical variables f and g and the commutator for the corresponding operators F and G, first noticed by Dirac in one of his brilliant insights (See Ref.[1]), namely

$$\{f, g\}_{\text{classical}} \quad \longrightarrow \quad i\hbar[F, G].$$

One has, in this manner, for instance, for the canonical variables p_j and q_k the Poisson bracket

$$\{p_j, q_k\} = \delta_{jk}$$

and for the canonical operators P_j and Q_k the commutator

$$[P_j, Q_k] = -i\hbar\delta_{jk},$$

Because of this it is tempting to add a third property to the definition of the quantization map (3)

$$[\mathcal{Q}(f), \mathcal{Q}(g)] = -i\hbar\mathcal{Q}(\{f, g\}), \;\; \forall f, g \in C_C^\infty(R^{2n}).$$

However, this assumption is too naive; the Groenewold-van Hove theorem states that even for the simple case of $\mathcal{M} = R^{2n}$ a quantization map $\mathcal{Q}$ with these three properties for all variables f and q does not exist (Refs.[2], [3]). What can be expected instead is a relation (3′) of the form

$$\{\mathcal{Q}(f), \mathcal{Q}(g)\}_{\text{qu}} = \hbar\mathcal{Q}(\{f, g\}_{\text{cl}}) + \ldots\ldots,$$

with higher order terms in $\hbar$ of the form

$$\hbar^n M_n(f, g)\,, \quad n = 1, 2, \ldots, \quad M_1(f, g) = \mathcal{Q}(\{f, g\}_{\text{cl}}),$$

in which the M_n are bilinear maps

$$M_n \;:\; C_C^\infty(R^{2n}) \times C_C^\infty(R^{2n}) \;\rightarrow\; B(\mathcal{H}),$$

in fact bidifferential operators on R^{2n}, like the Poisson bracket.

The definition of quantization just given is general and makes sense for any classical mechanic system with as phase space a symplectic manifold $(\mathcal{M}, \omega)$.

For $\mathcal{M} = R^{2n}$ we have the irreducible system of canonical operators P_j and Q_k as differential en multiplication operators in the usual Schrödinger representation. According to the theorem of Stone and von Neumann this system is unique, up to unitary equivalence. Let us, for the sake of simplicity of notation, take $n = 1$. Quantization then means a rule for assigning an operator to each classical monomial $p^m q^n$. This is sufficient; the quantization of more general functions can be found by taking appropriate limits of polynomials in p and q. It is immediately clear there are more than one way to do this. Classically $pq = qp$, but in quantum theory $PQ \neq QP$, so in quantum theory this may give

$$\mathcal{Q}_1(pq) = \frac{1}{2}(PQ + QP),$$

or

$$\mathcal{Q}_2(pq) = \frac{i}{2}(PQ - QP).$$

There is a priori no reason to prefer the one above the other. Quantization of a given classical system involves a choice; it is not unique. Note that

$$\mathcal{Q}_1(pq) - \mathcal{Q}_2(pq) = QP + \frac{1}{2}(1+i)1_{\mathcal{H}} + \frac{1}{2}(1-i)\hbar\, 1_{\mathcal{H}},$$

which shows that the appearance in the formula for quantization of terms of higher order in $\hbar$ is quite natural. Here is another example: one has $pq^4p = q^2p^2q^2$ but $PQ^4P \neq Q^2P^2Q^2$ with a difference

$$PQ^4P - Q^2P^2Q^2 = 2\hbar^2Q^2.$$

Note that in all the operators P and Q are unbounded, defined on dense linear subspaces of $\mathcal{H}$. This means that some care is needed in algebraic manipulation of these operators. This can be taken care of by defining some common dense domain on which these manipulations are permissible. We shall not worry about this. In the next sections we shall discuss two examples of quantization prescriptions.

5.3. Born-Jordan quantization

Max Born and Pascual Jordan published in 1925 an article (Ref.[4]) in which they extensively commented on a paper on quantum mechanics, just published at that time by Heisenberg (Ref.[5]), in fact one of the founding papers of the subject. They observed in particular that Heisenberg's algebraic noncommuting variables p_j and q_k were in fact infinite matrices. From then onwards Heisenberg's formulation of quantum mechanics became known as *matrix mechanics*. What interests us here is that they put forward a quantization prescription for arbitrary monomials $q^m p^n$

$$q^m p^n \;\;\rightarrow\;\; \frac{1}{n+1}\sum_{k=0}^{n} P^{n-k}Q^m P^k.$$

Their argument for this is part of long discussion and reformulation of Heisenberg's results and is therefore not easy to summarize.

5.4. Weyl quantization 1

Another prescription which eventually surpassed that of Born and Jordan in popularity was put forward in 1927 by Hermann Weyl (Ref.[6]). Weyl gave a general Fourier integral formula, to be discussed in the next section, from which a prescription for polynomials can be derived. This integral formula emerged later in mathematics as a particular way of defining *pseudodifferential operators*, a topic of great interest, although it has not much to do with quantum theory or quantization. Weyl's prescription for the quantization of arbitrary monomials, a result of his integral formula, reads

$$q^m p^n \;\;\rightarrow\;\; \frac{1}{2^n}\sum_{k=0}^{n} \frac{n!}{(n-k!)k!} P^{n-k}Q^m P^k.$$

The Born-Jordan and the Weyl quantizations are different, but only for $m > 1$, $n > 1$. One verifies easily

$$qp \;\;\rightarrow\;\; \frac{1}{2}(PQ + QP),$$

for both Born-Jordan and Weyl. One has however, for Born-Jordan

$$q^2 p^2 \;\;\rightarrow\;\; \frac{1}{3}(P^2Q^2 + PQ^2P + Q^2P^2),$$

and for Weyl

$$q^2p^2 \;\rightarrow\; \frac{1}{4}(P^2Q^2 + PQ^2P + Q^2P^2).$$

The only physically realistic case in which products of position and moment variables occur is that of a particle with electric charge e moving in a given magnetic potential $\vec{A}(\vec{x})$, in which the Hamiltonian is

$$H = \frac{1}{2me}\left(\vec{p} + \frac{e}{c}\vec{A}\right) \cdot \left(\vec{p} + \frac{e}{c}\vec{A}\right),$$

with the vector potential $\vec{A}$, connected to the magnetic field strength B through

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

or written explicitly in components

$$B_1(\vec{x}) = \frac{\partial}{\partial x_2}A_3(\vec{x}) - \frac{\partial}{\partial x_3}A_2(\vec{x}),$$

$$B_2(\vec{x}) = \frac{\partial}{\partial x_3}A_1(\vec{x}) - \frac{\partial}{\partial x_1}A_3(\vec{x}),$$

$$B_3(\vec{x}) = \frac{\partial}{\partial x_1}A_2(\vec{x}) - \frac{\partial}{\partial x_2}A_1(\vec{x}).$$

This means that for all practical purposes both quantizations can considered to be physically equivalent. In any case, when there are different quantizations for some classical expression, physical experiments should decide which one is the correct one.

5.5. Weyl quantization 2. An integral formula

Weyl's quantization formula, a particular kind of integral formula, first presented both in a paper (Ref.[6]) and in his famous book (Ref.[7]), was clearly suggested by his interest in applying group theory to quantum physics, a subject that he pioneered. See for his active interest in the new quantum mechanics Ref.[8]. (Note in passing that he also wrote one of the first books on general relativity (Ref.[9]), so here we have again a mathematician with great interest in and knowledge of physics).

His arguments for choosing his quantization formula are not easy to follow, but the resulting formula's are elegant and clear. One

of the things that bothered him was the sloppy way his physics colleagues treated the canonical operators P_j and Q_k, unbounded operators which cannot simply be added and multiplied with each other because of domain problems. For this reason he proposed to use instead the exponentiated forms, the 1-parameter unitary groups $U(\alpha) = e^{\frac{i}{\hbar}\alpha P}$ and $V(\beta) = e^{i\beta Q}$. They satisfy the commutation relation

$$U(\alpha)V(\beta) = e^{i\alpha\beta}V(\beta)U(\alpha)\,.$$

or

$$e^{\frac{i}{\hbar}\alpha P}e^{i\beta Q} = e^{i\alpha\beta}e^{i\beta Q}e^{\frac{i}{\hbar}\alpha P}\,.$$

which is the rigorous form of the usual commutation relation

$$[P, Q] = -i\hbar 1_{\mathcal{H}}.$$

The operators $U(\alpha) = e^{\frac{i}{\hbar}\alpha P}$ and $V(\beta) = e^{i\beta Q}$ can be combined to form what is nowadays called the *Weyl operator*

$$W_\hbar(\alpha, \beta) = e^{-\frac{1}{2}\alpha\beta}e^{\frac{i}{\hbar}\alpha P}e^{i\beta Q},$$

which can also be written as

$$W_\hbar(\alpha, \beta) = e^{\frac{i}{\hbar}(\alpha P+\beta Q)},$$

which is in fact a definition of the right hand side, because a linear combination $\alpha P+\beta Q$ of the two noncommuting selfadjoint operators P and Q is a priori not well defined.

The notion of *Weyl operator* and in particular 'Weyl system' has been championed by Irving Segal who used it as basis for his work on the mathematical foundations of quantum field theory. See Ref.[10]. It is for the canonical operators formulated in this exponential Weyl form that the Stone-von Neumann uniqueness theorem holds.

Note that I include in all formulas Planck's constant. The mathematical literature usually does not do this. The point of view here is that quantum mechanics is a deformation of classical mechanics, with $\hbar$ as deformation parameter. So $\hbar$ should be visible.

The argument from Weyl's 1927 paper on quantum theory (Ref.[5]) and also from his book (Ref.[6]), leading to his formula for (relatively) arbitrary functions of the operators P and Q, can be summarized as follows, again for the 1-dimensional case, to keep the noation simple :

Let $f(p,q)$ be a classical function on the (2-dimensional) phase space R^2. The aim of Weyl's procedure is to assign to this an operator function $f(P,Q)$ in the Hilbert space $L^2(R^1,dx)$. The usual Fourier transformation in quantum mechanics connects the 'position representation' with the 'momentum' representation, i.e. $\mathcal{H}=L^2(R^1,dx)$ with $\widehat{\mathcal{H}}=L^2(R^1,dp)$, according to the formulas

$$\widehat{\psi}(p)=\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{+\infty}\psi(x)e^{-\frac{i}{\hbar}px}\,dx,$$

and its inverse

$$\psi(x)=\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{+\infty}\widehat{\psi}(p)e^{+\frac{i}{\hbar}px}\,dp.$$

Here we do something different. We start with square integrable functions $f(p,q)$ on the phase space and transform these to a space $\mathcal{H}'=L^2(R^2,du\,dv)$ according to

$$\widehat{f}(u,v)=\frac{1}{2\pi\hbar}\iint f(p,q)e^{-\frac{i}{\hbar}(up+vq)}dp\,dq,$$

with inverse

$$f(p,q)=\frac{1}{2\pi\hbar}\iint \widehat{f}(u,v)e^{\frac{i}{\hbar}(up+vq)}du\,dv.$$

Weyl's definition of the operator $f(P,Q)$ simply employs the last formula, rewrites it as an operator formula, uses the second form of the formula for $W_\hbar(\cdot,\cdot)$, which gives

$$f(P,Q)=\frac{1}{2\pi\hbar}\iint \widehat{f}(u,v)e^{\frac{i}{\hbar}(uP+vQ)}du\,dv=$$

$$=\frac{1}{2\pi\hbar}\iint \widehat{f}(u,v)\,e^{-\frac{i}{2}\alpha\beta}e^{\frac{i}{\hbar}\alpha P}e^{i\beta Q}du\,dv.$$

Of, course whether this operator $f(P,Q)$ is well-defined depends on the properties of the numerical function $f(p,q)$. A nontrivial matter which has to be investigated carefully. Weyl's integral formula defines what is now called a *pseudodifferential operator* in $L^2(R^1,dx)$.

By choosing $f(p,q)=p^mq^n$ one finds Weyl's prescription for the quantization of monomials.

A question that remains is whether Weyl's quantization idea can be applied to a classical system for which the phase space is not R^{2n}

but an arbitrary symplectic manifold $\mathcal{M}$. No answers are known to me. Covering $\mathcal{M}$ by local Darboux coordinate systems?

5.6. Strict deformation quantization

Planck's constant $\hbar$ appeared in all the quantum formulas in the preceding discussions. This was to emphasize the idea that quantum theories are em deformations of classical theories, with $\hbar$ as deformation parameter. Note that $\hbar$ is a constant of nature. Choosing units for physical variables will change the *numerical value* of $\hbar$. If we use the kilometer as unit of length this numerical value becomes vanishing small; we are approaching the *classical limit* of the quantum system. In this and the next section we shall discuss explicit ways in which this idea of deformation quantization has been expressed.

In the first place there is *strict deformation quantization*, an attempt to construct for a given symplectic manifold a quantized system, analytically dependent on $\hbar$. This has been undertaken by Marc Rieffel (Refs.[11], [12]). He starts from a commutative C^*-algebra $\mathcal{A}$ of continuous functions on a given symplectic manifold $\mathcal{M}$. In $\mathcal{A}$ he define a deformation, depending on $\hbar$, of the given algebra multiplication, together with a deformation both of the norm and of the $*$-operation on $\mathcal{A}$. In this manner he obtains a *field* of noncommutative C^*-algebras $\{\mathcal{A}_\hbar\}_{\hbar\in R^1}$. He has obtained interesting rigorous results for several manifolds $\mathcal{M}$, none of which is however of particular physical interest.

5.7. Formal deformation quantization

5.7.1. Introduction

The difficulties of obtaining rigorous results, as is obvious from the work of Rieffel, has led to work on 'approximate deformation' quantization in which one looks at deformation quantization in term of a power series in $\hbar$, not necessarily convergent. If one goes only up to first order this is called *first order* or *infinitesimal* deformation quantization. The case of infinite power series, to be discussed in this section, is called *formal deformation quantization*.

Formal deformation quantization as a subject was initiated in 1977 in a letter and in 1978 in two long and fairly complicated papers by

what might be called the 'Dijon School', BBFLS in alphabetic order, the physicists Moshé Flato(†1998) – its de facto leader, François Bayen, Christian Fronsdal, Daniel Sternheimer from Dijon, together with the differential geometer André Lichnerowicz(†1998) from the Collège de France in Paris. Refs.[13],[14]. This work went unnoticed for several years, but then started to draw attention; more and more papers were written developing the ideas of what then indeed became to be known as 'formal deformation quantization', a true avalanche, culminating in the work of Fedosov and finally Kontsevich with his formality theorem, for which he, among other things, was awarded a Fields Medal in 1998.

The original intention of BBFLS was to find a description of quantum mechanics which was to be an alternative to the standard Hilbert space formalism, incorporating Dirac's idea of the connection between the classical Poisson bracket and the quantum commutator, dependent on Planck's constant $\hbar$ as a deformation parameter. However this approach developed gradually into an independent mathematical field, of great interest, but with less and less relevance to physics, something that may remind us of what happened to ergodic theory, started as an attempt to lay a basis for classical statistical mechanics, later independently developed into a general theory of the asymptotic behaviour of groups of measure preserving transformations.

The main idea of this approach is to avoid difficult problems of functional analysis by working with formal power series, leaving aside the questions of their convergence. A certain justification for this can be found in the fact that it is not unusual in physics to work with asymptotic series. In any case, this makes it mathematically into a problem of algebra.

So instead of trying to find a strict deformation of the algebra of classical observables, one constructs a larger auxiliary algebra of formal power series in the deformation parameter $\hbar$, with coefficients in the classical algebra, on which a deformed (noncommutative) product, a so-called *star product* is defined.

This idea of formal deformation quantization is based on the work of Gerstenhaber on the formal deformation of associative algebras (Ref.[13]).

5.7.2. The Gerstenhaber deformation formalism

Let $\mathcal{A}$ be a given associative algebra, over $\kappa = R, C$, with unit element. A formal deformation of $\mathcal{A}$ is given by an infinite series of bilinear maps

$$\phi_n \ : \mathcal{A} \times \mathcal{A} \ \longrightarrow \ \mathcal{A}, \ \ (a, b) \ \ \mapsto \ \phi_n(a, b), \ \forall a, b \in \mathcal{A}.$$

These maps are supposed to define a deformation $\bullet_\lambda$ of the multiplication $(a, b) \mapsto ab$ in the algebra $\mathcal{A}$, according to the infinite power series

$$a \bullet_\lambda b = ab + t\phi_1(a, b) + t^2\phi_2(a, b) + \ldots .$$

This series is formal; whether it converges or not for certain values of the parameter λ is irrelevant in this context. Such questions may be asked in the search for strict deformations. It involves functional analysis, as in the work of Rieffel. Here we are concerned with purely algebraic methods.

One may nevertheless ask what the precise mathematical meaning of such a formal power series is. There is an elementary answer. A formal series can be seen as an infinite sequence of elements of $\mathcal{A}$

$$\widehat{a} = (a_0, a_1, a_2, \ldots),$$

These sequences form a linear space, and in fact an associative algebra with respect to the multiplication

$$\widehat{a}\widehat{b} = (a_0b_0, \ a_0b_1 + a_1b_0, \ a_0b_2 + a_1b_1 + a_2b_0, \ldots),$$

or

$$(\widehat{ab})_0 = a_0b_0, \ \ (\widehat{ab})_1 = a_0b_1 + a_1b_0, \ldots \ ,$$

a multiplication which is in fact an extension of the given multiplication on $\mathcal{A}$. This idea can be given a slightly more sophisticated form by calling this extended algebra the algebra of formal power series in the indeterminate λ, with coefficients in $\mathcal{A}$. As such it is usually denoted as $\mathcal{A}[[\lambda]]$. We shall not worry about this and use the power series, looking at the λ, in this context just a bookkeeping device.

The deformed product need to be associative, which means

$$(a \bullet_\lambda b) \bullet_\lambda c = a \bullet_\lambda (b \bullet_\lambda c), \quad \forall a, b, c \in \mathcal{A}.$$

Writing this out as power series and comparing terms of the same order gives a series of conditions. In first order one finds

$$a\phi_1(b,c) - \phi_1(ab,c) + \phi_1(a,bc) - \phi_1(a,b)c = 0, \quad \forall a,b,c \in \mathcal{A}.$$

For general order n one gets, by an elementary but long calculation

$$a \bullet_t \phi_n(b,c) - \phi_n(a \bullet_t b, c) + \phi_n(a, b \bullet_t c) - \phi_n(a,b) \bullet_t c =$$

$$= \sum_{i=1}^{n-1} \{-\phi_{n-i}(a, \phi_i(b,c)) + \phi_{n-i}(\phi_i(a,b), c)\}.$$

This is at it stands a rather messy set of conditions. It can be brought in a mathematically elegant form by invoking *cohomology theory*, a broad set of mathematical ideas, which are, however, outside the scope of these lectures.

There is an equivalence relation between deformations. It is based on the following general idea. Suppose that we have a vector space V which is an associative algebra $\mathcal{A}_1$ with multipication $\bullet_1$, and suppose that we have an invertible linear map from V onto itself. We then can use T to define a new multiplication $\bullet_2$ on V by

$$a \bullet_2 b = T^{-1}(T(a) \bullet_1 T(b)).$$

This makes V into an associative algebra $\mathcal{A}_2$. The map T is an algebra isomorphism from $\mathcal{A}_1$ onto $\mathcal{A}_2$. If two formal deformations of $\mathcal{A}$, $\{\phi_n^{(1)}\}_{n=1,2,\ldots}$ and $\{\phi_n^{(2)}\}_{n=1,2,\ldots}$, are connected by a sequence of linear maps $\{T_n\}_{n=1,2\ldots}$ such that

$$T_n(\phi_n^{(2)}(a,b)) = \phi_n^{(2)}(T_n(a), T_n(b)), \quad \forall a,b \in \mathcal{A},$$

then the deformations are equivalent. The sequence $\{T_n\}_{n=1,2\ldots}$ is a formal linear map $\mathcal{A} \longrightarrow \mathcal{A}$. A deformation which is equivalent to the identity deformation is called trivial. Also this has an elegant cohomological formulation, which we cannot discuss in these lectures.

Application of the Gerstenhaber deformation formalism op formal deformation quantization is simple.

The algebra $\mathcal{A}$ becomes $C^\infty(\mathcal{M})$, for a given symplectic manifold $\mathcal{M}$, the phase space of a classical mechanical system. A formal deformation is given by a sequence of bilinear maps

$$\mathcal{A} \times \mathcal{A} \longrightarrow \mathcal{A},$$

which we may denote as $M_n(\cdot,\cdot)$. For $n=1$ we have

$$M_1(f,g) = i\{f,g\},$$

with the Poisson bracket $\{f,g\}$ on $C^\infty(\mathcal{M})$. In words : a deformation quantization *'in the direction of the Poisson bracket'*. A sequence $\{M_n\}_{n=1,2...}$ indeed determines in principle a formal deformation quantization. Two deformation quantizations may be equivalent. A deformation equivalent to the unit deformation is called *trivial*.

The deformation parameter λ becomes Planck's constant $\hbar$. The deformed product – the famous *'star product'* of the Dijon School – is denoted as $*_\hbar$.

There is one additional condition, namely that all the bilinear maps M_n are bidifferential operators on $C^\infty(\mathcal{M})$, just as the Poisson bracket.

One more point has to be taken care of. Our commutative classical algebra is the algebra $\mathcal{A} = C_C^\infty(\mathcal{M})$ of complex-valued smooth functions on $\mathcal{M}$; the deformed quantum algebra $\mathcal{A}_\hbar$ a complex $*$-algebra (or algebra with involution). Because of this a few additions have to be made to the formalism. This is left to the reader.

All this together in principle settles the questions of the criteria for existence and equivalence of formal deformation quantizations. To actually construct such quantizations is quite another matter. Much of the abundant literature on formal deformation quantization is in various ways devoted to this.

The initial aim of the founders of the 'Dijon School' was to develop an alternative approach to quantum theory, without Hilbert space and operators, as they explicitly write in the introduction of their first paper (Ref.[13]). However, the subject became more and more pure mathematics, with such high points as the work of Fedosov (Ref.[14]) and Kontsevich (Ref.[15]), as such of great interest, but with less and less relevance to physics. It should be noted however that the proof of the 'formality theorem' of Kontsevich has as an important input the method of Feynman diagrams from quantum field theory.

5.8. Concluding remarks

Neither strict deformation quantization (Rieffel) nor formal deformation quantization (Dijon school) are quantizations in the precise sense of the definition we gave in Section 5.2. In both cases there is a symplectic manifold as classical phase space, algebras of functions on this manifold, representing the classical observables, but no quantum Hilbert space with selfadjoint operators, so no assignment of such operators to classical variables.

There is in both approaches a problem of identification of the quantum observables. There is only one space, the commutative algebra of classical observables. It is clear which elements represent the classical p_j, q_k and the quantum P_j, Q_k. But what about $p_jq_k = q_kp_j$, P_jQ_k and Q_kP_j? All three are different; the two quantum variables depend moreover on $\hbar$. This question does not seem to have been discussed.

5.9. References

[1]. P.A.M. Dirac
The Fundamental Equations of Quantum Mechanics
Proceedings of the Royal Society London), A109, 642-653 (1925)

[2]. H.J. Groenewold
On the principles of elementary quantum mechanics
Physica 12, 405-460 (1946)

[3]. L. van Hove
Sur certaines représentations unitaire d'un groupe infini des transformations
Mémoire de l'Académie Royales des Sciences de Belgique 26, 1-102 (1951)

[4]. M. Born, P. Jordan
Zur Quantenmechanik
Zeitschrift fü Physik 34, 858-888 (1925)

[5]. Werner Heisenberg
Über die quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen
Zeitschrift für Physik 33, 879-893 (1925)

English translation in
Sources of Quantum Mechanics

B.L. van der Waerden, editor
Dover 1968

[6]. H. Weyl
Quantenmechanik und Gruppentheorie
Zeitschrift für Physik 46, 1-46 (1927)

[7]. Hermann Weyl
The Theory of Groups and Quantum Mechanics
(Translated from the 2d revised German edition 1931
Gruppentheorie und Quantenmechanik)
Dover 2003

[8]. Erhard Scholz
Weyl entering the 'new' quantum mechanics discourse
Contribution to the Conference
"History of Quantum Physics", Berlin, July 2-6, 2007. Accessible at:
`http://www2.math.uni-wuppertal.de/~scholz/preprints/HQ_1_ES.pdf`

Weyl's collected works were published in 1968 by Springer, translated into French in 1980, also publshed by Springer.

[9]. Hermann Weyl
Raum, Zeit, Materie
Springer, various editions
Translated from various editions as
Space, Time, Matter
Dover 1952

[10]. I.E. Segal
Representations of the canonical commutation relations
Lectures given at the 1965 Cargèse Summer School
Notes by P.J.M. Bongaarts and Th. Niemeijer
In "Applications of Mathematics to Problems
in Theoretical Physics", p.107-170
Marice Lévy, F. Lurcat, Editors
Gordon and Breach 1967

[11]. Marc A. Rieffel
Deformation Quantization and Operator Algebras
Proceedings of Symposia in Pure Mathematics 51, 411-423 (1990)

Available at::
http://math.berkeley.edu/~rieffel/
papers/deformation.pdf

[12]. Marc A. Rieffel
Deformation Quantization and C^*-Algebras
Contemporary Mathematics 167, 67-97 (1994)
Available at:
http://math.berkeley.edu/~rieffel/
papers/quantization.pdf

[13]. F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, D. Sternheimer
Quantum Mechanics as a Deformation of Classical Mechanics
Letters in Mathematical Physics 1, 521-530 (1977)

[14]. F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, D. Sternheimer
Deformation Theory and Quantization
I. Deformation of Symplectic Structures
Annals of Physics 111, 61-110 (1978)
II. Physical Applications
Annals of Physics 111, 111-151 (1978)

[15]. Murray Gerstenhaber
On the deformation of rings and algebras I, II
Annals of Mathematics 79, 59-103 (1963), 84, 1-19 (1966)

[16]. Boris V. Fedosov
A simple geometrical construction of deformation quantization
Journal of Differential Geometry 40, 213-238 (1994)
Available at:
http://intlpress.com/JDG/archive/1994/40-2-213.pdf

[17]. Maxim Kontsevitch
Deformation of Poisson Manifolds
Letters in Mathematical Physics 66, 157-216 (2003)
Obtainable at :
http://arxiv.org/abs/q-alg/9709040

• Reference added in this revised version of the text:

Chiara Esposito
Formality Theory: From Poisson Structures to Deformation Quantization
Springer 2014

6. Quantum Theory and Relativity

6.1. Introduction

Two new physical theories changed twentieth century physics in a dramatic way: quantum theory and the theory of relativity. The relation between the two is still far from clear; in their present form they are in a fundamental way incompatible with each other. In fact, to understand this is one of the main challenges for fundamental physics today.

So far in these lectures I have explained the basics of nonrelativistic quantum mechanics. In this lecture the road will be sketched to a relativistic version of the theory and the beginning of what is at this time the preliminary endpoint of this road, relativistic quantum field theory, a theory full of imperfections, even serious problems, in particular in its mathematical structure, but nevertheless very successful as a physical theory because it is able to predict experimental results with great accuracy.

In the twenties, when quantum mechanics in the form we know it now emerged over a short period of a few years, Einstein's theory of relativity, in particular his theory of special relativity, was already generally accepted as a universal theoretical framework for the physical world, even though it was realized that its consequences in terrestrial physics could only be expected to show up in situations in which very high velocities, approximately the velocity of light, would be involved, velocities that could at that time not be realized in experiments. The theoretical need for a relativistic version of quantum theory was nevertheless almost immediately felt and work started on it.

6.2. Einstein's special theory of relativity

Einstein wrote the fundamental paper in which he introduced his theory of relativity in 1905 (Ref.[1]), his 'Annus Mirabilis', the year in which he published five groundbreaking papers. His aim was to solve a problem related to motion and Maxwell's theory of electromagnetism, as is clear from the title of the paper (in English) : "On the Electrodynamics of Moving Bodies". This was connected with the problem of the *aether*, a substance which was supposed to fill the cosmos, serving as the carrier of electromagnetic waves,

and having very contradictory properties. The problems connected with this had already been under discussion by various nineteenth century physicists and mathematicians, such as Lorentz, FitzGerald and Poincaré.

One of these problems was the propagation of light as an electromagnetic wave. One would expect that its speed would depend on the motion of the earth through the aether. In 1889 Michelson and Morley showed by a very ingenious and precise interferometer experiment that there was no such dependence. The speed of light was always the same. Special relativity, in fact, solved this problem by simply abolishing the concept of aether altogether. Einstein later developed his general theory of relativity, a new description of gravitation.

The basic notion of classical Newtonian mechanics is that of an *inertial system*, a system of Euclidean coordinates in which a body not subjected to forces of any kind is either in rest or in rectilinear motion with constant velocity. This is connected with the following important principle assumed to be generally valid:

All inertial systems are physically completely equivalent; there is no preferred inertial system.

Acccording to Einstein the principle of inertia still holds, but it has to be interpreted in a new way. In the classical picture space is a 3-dimensional Euclidean vector space. Strictly speaking, it is an affine space, roughly a vector space in which the origin is irrelevant and can be chosen at will, a fine point that we shall not worry about. Time is an *external parameter* which describes the motion of a system in this space. In relativity theory time is not an separate variable; it is part of *spacetime*, a 4-dimensional affine space. What in this is time and what is space depends on the position of the observer.

This can be illustrated by looking at coordinate transformations. Let L be a given inertial system with spatial coordinates x, y, z. Consider a second inertial system L' with coordinates x', y', z', moving with respect to L with constant velocity v in the positive x-direction. In the nonrelativistic point of view this means that there is a coordinate transformation

$$x' = x - vt, \qquad y' = y, \qquad z' = z, \qquad (t' = t).$$

This is called a *Galileo transformation*. All such transformations for all possible velocities and in all possible directions, together with all rotations in space, form a group, the *inhomogeneous Galileo group*. If we also allow shifts of the origin of both position coordinates and time, it becomes the *inhomogeneous Galileo group*, the symmetry group of classical mechanics. We say that classical nonrelativistic mechanics is *Galileo covariant* and that its equations are *Galileo invariant*.

Einstein's great new idea was that one should not use Galileo transformations for going from one inertial system to another, but instead so-called *Lorentz transformations*. For the same case as above they are

$$x' = \gamma(x - vt), \qquad y' = y, \qquad z' = z, \qquad t' = \gamma(t - vx/c^2),$$

with $\gamma = (1 - v^2/c^2)^{-1/2}$ and c the velocity of light.

Two things should be noted in these formulas.

(1) This is not a 3-dimensional transformation, with t as an external parameter, but a truly 4-dimensional one. It indicates that we live in a 4-dimensional spacetime, with no absolute separation between space and time. What is space and what is time depends on the observer, a point that can be nicely illustrated by a 2-dimensional diagram, as we shall show further on. Mathematically a sequence of 4 numbers can always be regarded as coordinates for an 4-dimensional space, but in physics more is required, for instance, that objects in this 'space' can be rotated in a meaningful way. This is the case in 3 dimensions for Galilean space, but not in 4. Motion in the Einsteinian case in 4 dimensions makes physically sense, as the diagrams in the appendix following this lecture will show.

Strangely enough the idea of a 4-dimensional spacetime is not due to Einstein but to the mathematician Hermann Minkowski, a number theorist, who gave a talk on this in 1908 and subsequently published it in a paper in 1909 in which the above 2-dimensional picture first appeared. Here is a quote from this :

"*The views of space and time which I wish to lay before you have sprung from the soil of experimental physics, and therein lies their strength. They are radical. Henceforth space by itself, and time by itself, are doomed to fade away into mere shadows, and only a kind of union of the two will preserve an independent reality*".

Minkowski was another of these early 20^{th} mathematicians who had a deep interest in contemporaneous physics and morover made important contributions to it.

See Ref.[2], and also for an interesting paper on the mathematical and physical context of Minkowski's work Ref.[3].

It took some time before Einstein saw the merit of this point of view and in of what is now known as the Minkowski diagram – see below – and is universally used in undergraduate teaching of special relativity.

Note that the in the limit of $c \to \infty$ Lorentz transformations become Galileo transformations: Newtonian mechanics is the limit for $c \to \infty$ of relativistic mechanics, which remains valid for small values of c, i.e. small in the sense of what we have on earth, under normal circumstances.

6.3. Minkowski diagrams

Before we go further in this we shall call in the help of a tool of great pedagogical value, the *Minkowski diagram*. This is a 2-dimensional picture of spacetime. The problems that we are discussing have to do with the relation between space and time. Therefore a picture with the x and t coordinates is sufficient.

Minkowski published this picture in 1909, three years after Einstein's first paper on relativity theory. It remains curious that Einstein him self did not think much of it; he preferred to express the ideas of relativity algebraically, in formulas. Much later he changed his opinion in this. By now the Minkowski diagram has become the standard tool in teaching special relativity to students, in their first year and later.

Look first at picture 1 in the appendix following this lecture. It shows *empty spacetime*, with the x-axis and the t-axis. In picture 2 we see dots A and B. These represent *events*; a person of particle at spacetime points (x_1, t_1) or (x_2, t_2). There are lines (1), (2 and (3), *world lines*, representing histories of persons or particles. Line (1) describes a particle in rest at a certain position in space, letting the time go by. Line (2) is a particle that moves with constant speed. Line (3 describes a particle that is at rest until a certain moment, and then starts moving in an accelerated motion.

The next pictures, 3 and 4, show the change in spacetime coordinate systems, for Galileo transformation and for Lorentz transformations. In the first picture the time axis does not change, in the second picture both coordinate axes have moved. This indicates that in this last case there is a true motion in spacetime as a whole, a kind of 'hyperbolic' rotation,

Let us now forget about Galileo transformations and Newtonian mechanics and concentrate on relativity theory. Look for this at picture 5. It shows the *light cone*, in this 2-dimensional picture given by the equation

$$c^2t^2 - x^2 = 0.$$

The collection of spacetime points with $c^2t^2 - x^2 \geq 0$, $t \leq 0$ is called the *backward* or *past light cone*, with $c^2t^2 - x^2 \geq 0$ and $t \geq 0$ we speak of the *forward* or *future light cone*. Note that the our pictures show the light cone based at the origin. We can imagine a light cone at every point of spacetime. The light cone has much to to with the notion of *causality* in spacetime.

In picture 6 we see again three world lines, (1), (2) and (3), all three rectilinear motions with constant velocity and all three passing to the space point $x = 0$ at time $t = 0$. Line (1) is the sort of motion that any of us could have; a motion with a velocity smaller than that of light. Line (2) represents a motion along the light cone, it could be a neutrino, a particle that is (still) supposed to travel with the velocity of light. Finally, line (3) is a *tachion*, a particle that moves faster than light. This would create difficult conceptual problems with causality, mixing past and present, so one generally believes that tachions do not exist. A recent neutrino experiment at CERN which claimed that neutrinos can move faster than light has finally been discredited.

Note that this picture, as we have drawn it, supposes that we use units for time and length such that c is close to 1, otherwise the light cone would be extremely flat. This can be remedied by using $x^0 = ct$ as fourth coordinate, as is usual in many discussions of special relativity and in all discussions of the general theory.

Problem: Write down the general Galileo transformation from a given system L to a the system L' moving with a velocity $\mathbf{v} = v_x, v_y, v_z$ with respect to the system L.

The velocity of light c is roughly equal to $300,000$ km/sec. Almost no moving terrestrial objects, with the exception of electrons in an atom or subatomic particles in accelerators, have a speed that comes near to this. The quotient v/c is very small and the factor γ is to a high precision equal to 1, which means that it is difficult to detect the difference between classical and relativistic mechanics.

Let us perform two successive Galileo transformations in the x-direction, with the velocity v_1 going from L to L' and v_2 from L' to L'', the resulting velocity v from L to L'' will be $v = v_1 + v_2$. This is different in Einstein's theory; one can calculate v there to be $v = (1 + (v_1 v_2)/c^2)^{-1/2}(v_1 + v_2)$.

Note that that for velocities much smaller than that of light also this formula is very close to the pre-Einstein formula.

Suppose that an object moves with a velocity u in the x direction of the inertial system L. Its velocity u' in L' is

$$u' = \frac{u - v}{1 - uv/c^2}.$$

By substituting $u = c$ one gets $u' = c$, i.e. the velocity of light is the same in different inertial systems, a fundamental feature of special relativity, in agreement with the results of the Michelson and Morley experiment.

One can show that the bilinear form

$$< (x, y, z, t), (x', y', z') >= c^2 tt' - (xx' + yy' + zz')$$

is invariant under Lorentz transformations. In fact Lorentz transformations can be defined as the linear transformations that leave this form invariant. They form a group sometimes denoted as $SO(1, 3)$ (pseudo-orthogonal group in 4 dimensions). For $t = t'$ it restricts to the standard positive definite Euclidean inner product of space – apart from an overall minus sign, but on spacetime as a whole it is indefinite; the corresponding 4-dimensional spacetime 'length' $(ct)^2 - (x^2 + y^2 + z^2)$ can be positive, negative or zero. Spacetime as a 4-dimensional vector space provided with this inner product is called *Minkowski space*.

Recommended reading for all this is a collection of the basic papers on relativity theory by, among others, Einstein, Minkowski and Lorentz, in English translation (Ref.[4]).

6.4. The Klein-Gordon equation

One of the basic features of special relativity is that space and time have to be treated on the same footing. The Schrödinger equation is clearly not relativistic; as a differential equation it is of first order in time and of second order in the space variables. Immediately after the appearance of the first papers on quantum mechanics a search for a relativistic analogue started. Schrödinger himself found such an equation but did not publish it because he was aware of its problematic aspects. Several others found the same equation and did publish it, among them Oskar Klein and Walter Gordon, after whom the equation was eventually named. It is not hard to prove that there exists no Lorentz invariant first order differential equation. The *Klein-Gordon equation* is a second order equation. For the description of a single free particle of mass m it reads

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \frac{m^2c^2}{\hbar^2}\right)\phi = 0.$$

Before studying this equation further we introduce notation which is convenient for all discussions in relativity, among other things because it brings out the 4-dimensional spacetime character of the theory, and is therefore used in most books on relativity and especially in books on relativistic quantum field theory. It is also important and even indispensable in general relativity, which involves differential geometry on manifolds, but this does not concern us here. We shall use the following conventions :

(1) We shall have spacetime coordinates $\{x^\mu\}_\mu$, with $x^1 = x$, $x^2 = y$, $x^3 = z$ and $x^0 = ct$. The symbol x will from now on mean the quadruple (x^0, x^1, x^2, x^3). Latin indices j, k, etc. are used for the spatial coordinates with $\mathbf{r} = (x^1, x^2, x^3)$.

(2) We use lower (covariant) indices and upper (contravariant) indices, as is usual in differential geometry.

(3) We employ the Einstein convention : summation signs are omitted when summing over the same index, one covariant, the other contravariant. Example : $x^\mu y_\mu$ for $\sum_\mu x^\mu y_\mu$.

(4) A Lorentz transformation Λ acts on the spacetime coordinates as a 4×4 matrix : $(x^\mu)' = \Lambda^\mu{}_\nu x^\nu$.

(5) The Minkowski inner product is written with the help of a covariant 'metric 2-tensor' g, with elements $g_{00} = 1$, $g_{jk} = -\delta_{jk}$, and with the other $g_{\mu\nu}$ being 0. So $< x, y >= g_{\mu\nu}x^\mu x^\nu$. Sometimes the converse (contravariant) 'metric 2-tensor' is used with the same elements $g^{\mu\nu} = g_{\mu\nu}$. This seems a bit trivial, but it facilitates the simple writing of various formulas. It also reflects the fact that special relativity can be seen as a locally linearized form of general relativity, a point which we shall not discuss here.

Problem: Show that these two tensors are each others inverses, by calculating $g^{\mu\rho}g_{\rho\nu}$.

(6) The partial derivative $\frac{\partial}{\partial x^\mu}$ is written as ∂_μ, with also $\partial^\mu = g^{\mu\nu}\partial_\nu$.

t Using these conventions the Klein-Gordon equation can simply be written as

$$(\partial^\mu\partial_\mu + m^2c^2/\hbar^2)\phi(x) = 0.$$

Note that in elementary particle theory one generally uses units such that $c = 1$ and $\hbar = 1$. In that context the equation becomes just

$$(\partial^\mu\partial_\mu + m^2)\phi(x) = 0.$$

Problem: Show that the Klein-Gordon equation is indeed Lorentz invariant, i.e. that if the function $\phi(x)$ is a solution than also the Lorentz transformed function $\phi'(x) = \phi(\Lambda^{-1}x)$.

The Klein-Gordon equation is a relativistic equation. However, can we use it as a quantum mechanical wave equation? It has two serious problems, probably the reason why Schrödinger did not publish it.

(1) The Schrödinger equation has a positive definite inner product. For a unit vector ψ one has $(\psi, \psi) = \int_{-\infty}^{+\infty}\rho(\mathbf{r})\, d\mathbf{r} = 1$ with $\rho(\mathbf{r}) = |\psi(\mathbf{r})|^2$ the positive normalized probability density for finding the particle at position $\mathbf{r}$, one of the basic facts of quantum mechanics. The normalization of the probability density is conserved in time. A similar expression $(\phi, \phi) = \int_{-\infty}^{+\infty}\phi(\mathbf{r})^*\phi(\mathbf{r})\, d\mathbf{r}$ for solutions for the Klein-Gordon equation is useless in this respect. The equation is second order in time, so for a solution one has to give as Cauchy data both ϕ and its time derivative $\dot{\phi}$. There is in this case only one mathematically reasonable sesquilinear expression, namely

$$(\{\phi_1, \dot{\phi}_1\}, \{\phi_2, \dot{\phi}_2\}) = i\int_{-\infty}^{+\infty}(\overline{\phi}_1\dot{\phi}_2 - \overline{\dot{\phi}_1}\phi_2)\, d\mathbf{r}.$$

This is however indefinite; the expression $(\{\phi,\dot{\phi}\},\{\phi,\dot{\phi}\})$ can be negative, as can be checked easily, and this excludes a probabilistic interpretation.

(2) The Fourier transform of a solution of the Klein-Gordon equations contains both positive and negative frequencies. This means that if we still want to use it as a quantum mechanical equation there will be particles with energies going to $-\infty$, which is unacceptable physically.

For these two reasons the Klein-Gordon equation is *physically* unacceptable as a Schrödinger type wave equation and has as such to be dismissed. As a *mathematical* equation it reappears in quantum field theory, however with a very different mathematical meaning, as a so-called *field operator* and associated with that, a very different physical interpretation.

6.5. The Dirac equation

There are no Lorentz invariant first order differential equations, that is to say not for *scalar* functions. It was Dirac's idea to look for first order equations for functions with more components. In 1928 (Ref.[8]) he proposed the following equation for a function

$$\psi\ :\ R^4 \to C^4,$$

written in his notation as

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[\beta mc^2 + i\hbar c\sum_{j=1}^{3}\alpha_j\frac{\partial}{\partial x^j}\right]\psi(\mathbf{r},t).$$

In this ψ has 4 complex components; there are three 4×4 matrices α_j and a single matrice β with the properties $\alpha^2=\beta^2=1$ and with all pairs of different matrices anticommuting. The matrix indices for the α_j and for β are omitted.

For the modern formulation we use the conventions introduced in the preceding section and moreover the so-called γ-*matrices* defined as

$$\gamma^0=\beta,\qquad \gamma^k=\beta\alpha_k,\ \ k=1,2,3.$$

These matrices satisfy the anticommutation relations

$$[\gamma^\mu,\gamma^\nu]_+ = 2g^{\mu\nu}.$$

This leads to a compact and elegant form of the Dirac equation, namely

$$(i\gamma^\mu \partial_\mu - mc/\hbar)\psi(x) = 0.$$

For units with $c = \hbar = 1$ it becomes $(i\gamma^\mu \partial_\mu - m)\psi(x) = 0$.

This form of the equation exemplifies the visible beauty of the equations of modern physics, in particular those of relativity theory, special and general. See Ref.[7].

The Dirac equation is a Lorentz invariant equation, which is a bit more difficult to see than in the case of the Klein-Gordon equation.

Reminder: Scalar functions on spacetime transform under Lorentz transformations as

$$\phi'(x) = \phi(\Lambda^{-1}x),$$

with the shorthand notation Λx meaning $(\Lambda x)^\mu = \Lambda^\mu{}_\nu x^\nu$. The Lorentz invariance of the Klein-Gordon equation means that if $\phi(x)$ is a solution then $\phi'(x)$ is also a solution. This is more complicated for the case of the Dirac equation.

In the first place we need the group $SL(2, C)$, the group of 2×2 complex matrices with determinant 1. It is the universal covering group of the Lorentz group $O(1, 3)$. Being the covering group of $O(1, 3)$ means that there is a two-to-one group homomorphism

$$g \mapsto \Lambda(g)$$

from $SL(2, C)$ onto $O(1, 3)$. We use a 4 dimensional representation of $SL(2, C)$. Note that both $SL(2, C)$ and $O(1, 3)$ are noncompact, which implies that all unitary representations of these groups are infinite dimensional.

The group $SL(2, C)$ acts on the 4-dimensional complex vector space spanned by the four components of ψ as

$$g \mapsto S(g),$$

a nonunitary matrix representation, while $O(1, 3)$ itself acts on the spacetime coordinates according to

$$(x')^\mu = \Lambda^\mu{}_\nu x^\nu.$$

This together gives the Lorentz transformation – or rather $SL(2, C)$ transformation – of ψ as

$$\psi'(x) = S(g)\psi(\Lambda^{-1}(g)x).$$

Problem: Explain why one has to use $\Lambda^{-1}(g)$ instead of $\Lambda(g)$ in this transformation formula.

Problem: Show that the Dirac equation is indeed invariant under these transformations, i.e. that solutions are transformed into solutions.

As with the Klein-Gordon equation we have to ask whether the Dirac equation is acceptable as a quantum mechanical mechanical wave equation. We shall see that it is much better in this respect but still not perfect.

(1) The Dirac equation does have a time-independent positive inner product

$$(\psi, \varphi) = \int_{-\infty}^{+\infty} \sum_{j=1}^{4} \overline{\psi}_j(\mathbf{r})\, \varphi_j(\mathbf{r})\, d\mathbf{r}.$$

By substituting in this expression a unit vector $\psi = \varphi$, one gets

$$\rho(\mathbf{r}) = \sum_j \overline{\varphi}_j(\mathbf{r})\, \varphi_j(\mathbf{r}),$$

which can be interpreted as a probability density for the position $\mathbf{r}$. There remain problems with the measurement of position for relativistic particles. Solutions have been proposed, none of these totally convincing.

(2) The Fourier transform of a solution contains positive and negative frequencies, just as for the Klein-Gordon equation, so we have the same problem with un physical negative energies. In a 1930 paper in which Dirac discussed this problem, he proposed an ingenious and imaginative heuristic solution for this problem (See Ref.[9]). According to Dirac the vacuum is filled with infinitely many negative negative energy particles. There may be a few 'holes' in this 'sea'. These should be regarded as positive energy particles, positively charged.

At the time of writing only three elementary particles were known, the electron, with negative electric charge, the proton, with positive charge and the neutron, electrically neutral – as the name suggests. Because of this Dirac believed that he had found an equation that described electrons and protons. In 1932 a new positively charged particle was discovered in cosmic radiation by Anderson. It had the same mass as an electron and was called a *positron*. Dirac now

realized that he had found an equation for the electron and the positron as its *antiparticle*. For this he received the Nobel prize in 1933, sharing it with Schrödinger.

The Dirac equation has more strong points :

(1) For a particle in an electromagnetic field an interaction term is added, which gives, again with $c = \hbar = 1$,

$$(i\gamma^\mu(\partial_\mu + ieA_\mu(x)) - m)\psi(x) = 0$$

in which e is the electric charge and $A_\mu(x)$ the electromagnetic 4-potential, appearing in the relativistic formulation of Maxwell's theory of the electromagnetic field. For the electron in the simplest model for the hydrogen atom, only $A_0(x)$ is nonzero; it is the Coulomb potential $e^2/\mathbf{r}$. The other three components describe a possible magnetic field. The eigenvalue - eigenfunction equation for the hydrogen atom can be solved, just like in the case of the Schrödinger equation. Forgetting the unphysical negative energy eigenvalues one gets the hydrogen spectrum with relativistic corrections. Lines are split; one obtains the so-called *fine structure* of the spectrum, with values in good agreement with experiments. In this way it is a definite improvement on the nonrelativistic Schrödinger equation.

(2) The electron spin is automatically included in the Dirac equation; there is no need to add it 'by hand' to the wave equation as is necessary with the nonrelativistic Pauli spin which is just added 'externally' in the Schrödinger theory.

However, notwithstanding these successes, the Dirac equation – and notwithstanding Dirac's ingenious 'hole theory' interpretation of it – eludes all attempts to give it a consistent and clear mathematical meaning as a single particle wave equation. In fact, Dirac's interpretation does hint at a *many-particle situation*. That is the direction in which we have to go to give a mathematically and physically satisfactory description of the behaviour of relativistic particles.

The Dirac equation, but also the Klein-Gordon equation and other relativistic equations will acquire a new life as equations for *field operators*, in the context of *relativistic quantum field theory*. This will be discussed briefly in the next section.

Note finally that a few physics textbooks contain useful reviews of relativistic quantum mechanics, for instance the book by Albert Messiah (*Quantum Mechanics*, volume 2, Chapter XX).

6.6. Relativistic quantum field theory

6.6.1. Introduction

In general fields are physical quantities with one or more components, depending on space and time variables, with an evolution in time prescribed by partial differential equations. We know many such fields, the electromagnetic field, a combination of electric and magnetic fields, evolving in time according to Maxwell's equations, Einstein's gravitational field. Phenomena like hydrodynamics, aerodynamics, elasticity and many others are also described by fields.

Historical the main one for fundamental physics was the electromagnetic field. It was understood that matter consisting of atoms and molecules was kept together by electric and magnetic forces transmitted by fields. It is therefore not surprising that the founders of quantum theory tried to find a quantized version of this field. One of the more fruitful ideas was to see an electromagnetic field as a collection of infinite many harmonic oscillators of all possible frequencies. As one knew how to quantize systems of oscillators this made sense. For a free field, i.e. a field in vacuum, not interacting with charges and current this was not hard to, even though this meant dealing with systems with an infinite number of degrees of freedom, a situation in which von Neumann's uniqueness theorem for the operators that satisfy the canonical commutator relations no longer holds. Attempts at constructing a quantized version of interacting systems started already in the late nineteen twenties with work by Paul Dirac. Work in further developing this run into serious problems: persistent infinities at each level of proposed theories. From a practical point of views these problems were overcome by a procedure called *renormalization*, invented partly independently by Feynman, Dyson, Schwinger and Tomonaga in the nineteen fifties. Renormalization theory is a method, ad hoc but effective, in which most infinities, divergent integrals in fact, can be made to cancel. All this without real understanding why this is so. However, as a way to test experimentally the predictions of quantum field theories it has turned out to be very successful. This is in particular

true for *quantum electrodynamics* the theory that describes the electromagnetic interactions between particles, where certain quantities can be calculated with a precision up to six or seven decimals. So renormalization theory has become a standard tool for elementary particle theory. Nevertheless, the true mathematical nature of the theory remains mysterious. Fifty years of hard work by competent mathematical physicists has not resulted in remedying this.

I shall not say much about the nature of this problem, neither shall I discuss the history of the subject from its beginning in the fifties up till now, except for a few remarks at the end. Instead I shall give an introduction to the rigorous mathematical formalism for the physically rather trivial situation of free fields, describing particles which do not interact which each other, as a starting point for attempts to include physically meaningful interactions, a subject that lays outside these lectures.

6.6.2. Quantum field theory as a many particle theory

Because of the high velocities involved, elementary particle physics is necessarily relativistic. The main reason that relativistic quantum mechanical equations fail is that they describe single particles. However, a characteristic aspect of elementary particle physics, or as it is usually called, high energy physics, is that particles can be created and annihilated.

Earlier in this lecture I discussed the Klein-Gordon equation as a first candidate for a quantum mechanical relativistic wave equation. As such it had to be abandoned. The second candidate, the Dirac equation was better, but still not good enough. These and other similar equations were use to describe single particles. It took some time before this was properly understood and that it was realized that the same equations could be used, with a completely different mathematical meaning and different physical understanding, to describe in a relativistic way, as quantum field equations, the many-particle situations appearing in elementary particle physics.

In the second lecture we have discussed the discussion of many-particle systems in quantum mechanics. The Hilbert spaces of systems of n nonidentical particles were described by n-fold tensor products of the Hilbert spaces of the separate particles, symmetric tensor products $\mathcal{H}_s^{(n)} = \otimes_s^n \mathcal{H}^{(1)}$ for bosons, and antisymmetric tensor products $\mathcal{H}_a^{(n)} = \otimes_a^n \mathcal{H}^{(1)}$ for fermions.

Quantum field theory describes processes in which particles can be annihilated or created. In high energy accelerators an electron and its antiparticle, a positron can collide, be annihilated, while giving rise to the creation of a photon, the particle that carries the quantized version of electromagnetic radiation. This means that we need a many-particle Hilbert space, the countably infinite direct sum of all the tensor product spaces. Such a space is called a Fock space after the Russian physicist V.A. Fock who in 1932 first introduced it. We have

$$\mathcal{H}_s^{\text{Fock}} = \oplus_{n=0}^{\infty}(\otimes_s^n \mathcal{H}^{(1)}),$$

for bosonic particles, and

$$\mathcal{H}_a^{\text{Fock}} = \oplus_{n=0}^{\infty}(\otimes_a^n \mathcal{H}^{(1)}),$$

for fermionic ones. A Fock space with its operators has an interesting mathematical structure, which was later better understood by J.M. Cook (ref.[11]).

6.6.3. Fock space and its operators

Fock spaces have a characteristic system of operators, *annihilation and creation operators*, names that suggest the physical role that they play, namely that of creating and annihilating particles, the possibility of which is a typical feature of elementary particle physics. Mathematically they are used to move up and down in the many-particle Fock space. As I shall discuss as example a field theory for bosonic particles only, I restrict myself to the bosonic case.

Let $\mathcal{H}^{(1)}$ be a given 1-particle Hilbert space, with elements f, g, etc.. We define *creation operators*, for every f in $\mathcal{H}^{(1)}$, as operators

$$a^*(f) : \mathcal{H}_s^{(n)} \rightarrow \mathcal{H}_s^{(n+1)}$$

by linear extension of

$$a^*(f)(f_1 \otimes \ldots \otimes f_n)_s = (f \otimes f_1 \otimes \ldots \otimes f_n)_s,$$

and *annihilation operators*, for every g in $\mathcal{H}^{(1)}$, as operators

$$a(g) : \mathcal{H}_s^{(n)} \rightarrow \mathcal{H}_s^{(n-1)}$$

by linear extension of

$$a(g)(f_1 \otimes \ldots \otimes f_n)_s =$$

$$= [(g, f_1)(f_2 \otimes \ldots \otimes f_n)_s + \ldots + (g, f_n)(f_1 \otimes \ldots \otimes f_{n-1})_s],$$

There is 1-dimensional 0-particle space $\mathcal{H}^{(0)}$, with a preferred state Ψ_0, the ground state or *vacuum state*. Each annihilation operator acts on Ψ_0 as $a(f)\Psi_0 = 0$. It is not hard to derive the following commutation relations, for all f and g in $\mathcal{H}^{(1)}$,

$$[a^*(f_1), a^*(f_2)] = [a(g_1), a(g_2)] = 0, \qquad [a(g), a^*(f)] = (g, f).$$

For the Fermion case one has similarly defined creation and annihilation operators, with a few additional minus signs in the action of the annihilation operators, and anticommutation instead of commutation relations.

6.6.4. The scalar quantum field

The simplest quantum field is the real scalar field, in which the Klein-Gordon equation acquires a second life. It describes a system of spin zero particles, electrical neutral, for example π^0-mesons, produced from other particles in accelerators, but also found in cosmic radiation. The really interesting situation in physics is one in which there are several different fields, describing different particles, interacting with each other, e.g. electrons and positrons, protons and neutrons. The free scalar field on its own is a pedagogical example. Free means in this context that there are no attracting or repulsive forces between the particles, and that they do not collide with each other. Its great advantage is that it can be formulated with complete mathematical rigour, unlike interacting quantum field theories which all suffer from very serious mathematical mathematical problems, withstanding their great success as physical theories. As we cannot enter into the subject of interacting quantum fields and their difficulties in a serious manner, the scalar field is an excellent model to understand at least the first steps in setting up quantum field theory.

For this the 1-particle Hilbert space $\mathcal{H}^{(1)}$ consists of functions $f(p)$, with the variable $p = (p^0, p^1, p^2, p^3)$ a 4-vector in momentum space, restricted to a *mass shell*, a hypersurface in this space defined by the relation $p^0 = \sqrt{((p^1)^2 + (p^2)^2 + (p^3)^2)^{1/2} + m^2}$, which is invariant under Lorentz transformations $p^\mu = \Lambda^\mu_\nu p^\nu$. In this p^0 is the energy, m the mass, sometimes called the restmass, and $\mathbf{p} = (p^1, p^2, p^3)$ the 3-momentum. Note that we have chosen units such that $c = \hbar = 1$,

as is usual in elementary particle physics. The operator $a^*(f)$ creates a particle with a momentum wave packet $f(p)$. One would like to create particles with a sharp momentum p with a creation operator $a^*(p)$. This is, strictly speaking, impossible, just as it is, again strictly speaking, impossible to have particle with an exact position. Nevertheless, we do this, for both cases, heuristically.

6.6.5. Intermezzo : the Dirac δ-function

The mathematical language of all the standard textbooks in quantum field theory is heuristic. This makes for transparency and elegance; the disadvantage is that real and serious mathematical problems become invisible. Because of this transparency we shall also use this language, even though the free scalar quantum field can be formulated in full mathematical rigour. The central notion of this heuristic language is that of the Dirac δ-function and its derivatives.

In his famous textbook on quantum mechanics Dirac proposed a function $\delta(x)$ with the following properties:

Let x_0 be an arbitrary point on the real line. Then

$$\delta(x) = +\infty, \qquad \delta(x) = 0, \quad x \neq x_0.$$

It can be integrated, for an arbitrary point x_0 on the real line,

$$\int_{-\infty}^{+\infty} \delta(x - x_0)dx = 1.$$

Integration with an arbitrary function g gives

$$\int_{-\infty}^{+\infty} \delta(x - x_0)g(x)dx = g(x_0).$$

The δ-function has also a derivative $\delta^{(1)}(x)$, defined by the integration property

$$\int_{-\infty}^{+\infty} \delta^{(1)}(x - x_0)g(x)dx = g^{(1)}(x_0),$$

and so on for higher derivatives. Similarly in higher dimensions.

Of course, such a δ-function does not exist in rigorous analysis. A proper mathematical realization of the idea of 'generalized functions' of this sort has been given in terms of functional analysis by Laurent Schwartz in his *distribution theory*. According to this

the δ-function is a continuous linear functional $\delta(g) = g(0)$, on a space of so-called *test functions* with the heuristic representation $\delta(g) = \int_{-\infty}^{+\infty} \delta(x)g(x)dx = g(0)$.

6.6.6. The scalar quantum field. Continued

With these ideas in mind we write

$$a^*(f) = \int_{-\infty}^{+\infty} a^*(p)f(p)\,\frac{d\mathbf{p}}{p^0},$$

and

$$a(g) = \int_{-\infty}^{+\infty} a(p)\,\overline{g(p)}\,\frac{d\mathbf{p}}{p^0},$$

with $\mathbf{p} = (p^1, p^2, p^3)$, and with the commutation relations for the heuristic operators $a^*(p)$ and $a(p)$ written as

$$[a^*(p), a^*(p')] = [a(p), a(p')] = 0, \qquad [a(p), a^*(p')] = p^0\delta(p - p').$$

Sets of heuristic formulas of this type, for all sorts of particles, bosonic, fermionic, with different masses and spins, form the basis of all further developments of relativistic quantum field theory that one can find in standard textbooks.

6.6.7. The scalar quantum field. The field operators

The scalar quantum field itself, a system of (heuristic) operators on space time, $\{\widehat{\phi}(x)\}_{x\in R^4}$, is defined by performing a Fourier transformation on a combination of the (heuristic) annihilation operators and (heuristic) creation operators

$$\widehat{\phi}(x) = \frac{1}{(2(2\pi)^3)^{1/2}} \int_{-\infty}^{+\infty} \left(a(p)\,e^{-ipx} + a^*(p)\,e^{+ipx}\right)\,\frac{d\mathbf{p}}{p^0}.$$

with again $\mathbf{p} = (p^1, p^2, p^3)$ and $x = (x^0 = t, x^1, x^2, x^3)$ and the p^0 in the numerator under the integral to make the formula manifestly Lorentz invariant. From this one derives the field equations

$$(\partial^\mu\partial_\mu + m^2)\widehat{\phi}(x) = 0,$$

just the Klein-Gordon equation, but now as an operator equation describing a many-particle system. There are canonical equal-time commutation relations

$$[\,\widehat{\phi}(\mathbf{x_1}, t), \widehat{\phi}((\mathbf{x_2}, t)] = [\,\widehat{\pi}(\mathbf{x_1}, t), \widehat{\pi}((\mathbf{x_2}, t)] = 0,$$

$$[\,\widehat{\pi}(\mathbf{x_1},t),\widehat{\phi}(\mathbf{x_2},t)] = -i\delta(\mathbf{x_1}-\mathbf{x_2}),$$

with $\mathbf{x_j} = ((x_j)^1,(x_j)^2,(x_j)^3)$, $(x_j)^0 = t$ and $\widehat{\pi}((\mathbf{x},t) = \frac{\partial}{\partial t}\widehat{\pi}((\mathbf{x},t)$, the 'canonical momentum' conjugate to $\widehat{\phi}(\mathbf{x},t)$. Note that we are obviously in the Heisenberg picture, in which the observables depend on time while the state vectors in $\mathcal{H}_s^{\text{Fock}}$ remain constant. The Hamiltonian operator for this quantum system is

$$H_0 = \int_{-\infty}^{+\infty}\left[\frac{1}{2}\widehat{\pi}^2 + \frac{1}{2}(\nabla\widehat{\phi}\cdot\nabla\widehat{\phi} + \frac{m^2}{2}\widehat{\phi}^2\right]d\mathbf{x},$$

with

$$\nabla = \left(\frac{\partial}{\partial x^1},\frac{\partial}{\partial x^2},\frac{\partial}{\partial x^3}\right).$$

The operator H_0 as the energy operator is a constant of the motion, so it is time-independent, even in the Heisenberg picture.

This heuristic formulation can be made rigorous by starting from creation and operators depending on square integrable functions on momentum space, in the spirit of Section 6.6.3, then rewriting the Fourier transformation and finally obtaining the field operator as a functional $\widehat{\phi}(f)$ on a linear space of test functions f on space-time. This means that the free scalar quantum field is a mathematically well-defined model. However, by doing this the elegance and transparency of the heuristic description is lost. We would also no longer see the similarity and the differences between the Klein-Gordon equation as a one-particle quantum mechanical wave equation with numerical solutions, not very successful in this role, and as a many-particle operator equation, completely acceptable in a mathematical and physical sense. The free scalar quantum field is, together with all other similarly constructed free quantum field theories, the Dirac quantum field theory, quantum electrodynamics, the point of departure for the general field theories for interacting particles.

I should note here that the free Maxwell quantum field, i.e. the electromagnetic quantum field, has peculiar features, which make it more difficult – but not impossible – to formulate it rigorously. This has to do with the fact that the proper description has to use the electromagnetic 4-potential field $\widehat{A}_\mu(x)$. It turns out, however, that it is impossible to combine manifest Lorentz invariance for the

operators $\widehat{A}_\mu(x)$ with definite positivity of the inner product of the space in which they operate, which means that this space $\mathcal{H}_A$ is not the true Hilbert space of the system. The potentials $\widehat{A}_\mu(x)$ are not the physical operators, but instead of this one has the so-called field tensor

$$\widehat{F}_{\mu\nu}(x) = \partial_\mu \widehat{A}_\nu(x) - \partial_\nu \widehat{A}_\mu(x)$$

which lives in the physical Hilbert space, a quotient space $\mathcal{H}_F$ of $\mathcal{H}_A$. See Ref.[17].

6.6.8. The scalar field with self interaction

The next step is a quantum field theory for scalar particles that interact with each other. A possible sort of interaction is given by the interaction Hamiltonian

$$H_I = \frac{1}{4}\int_{-\infty}^{+\infty} \widehat{\phi}^4 d\mathbf{x}.$$

Together with the Hamiltonian of the free theory this gives a total Hamiltonian

$$H = H_0 + \lambda H_I,$$

with λ a so-called couplings constant. This leads to the nonlinear field equation

$$(\partial^\mu \partial_\mu + m^2)\widehat{\phi}(x) + \lambda\, \widehat{\phi}^3(x) = 0$$

By using the Fourier formula for $\widehat{\phi}(x)$ one can write H_0 as an expression in annihilation and creation operators in the Fock Hilbert space. This leads to a well-defined selfadjoint operator. It is unbounded, but has a perfectly acceptable dense domain of definition. This is not the case for the interaction Hamiltonian H_I. It can be also be written as a creation and annihilator expression, but this expression carries all the vectors of the Fock Hilbert space into 'nonnormalized' vectors, meaning that the domain of definition of this expression as an operator only contains the zero vector.

Elementary particle physicists do not worry about the mathematical existence of this and other similar formal operator expressions. They just use them as point of departure for perturbative calculations of processes between various particles. The terms of the resulting power series expansions all lead to divergent integrals. These

divergencies are removed by the systematic prescriptions of *renormalization theory*. The final results are finite and give excellent predictions for the outcomes of experiments. A rigourous mathematical basis for this still does not exists.

6.6.9. Final remarks

Quantum field theory is a curious theory. Quantum field theory was begun by Dirac in the nineteen twenties, run into the difficulties of infinities, was in the nineteen fifties in a practical sense revived as renormalized quantum electrodynamics through the work of Feynman and others and reached in the nineteen sixties its greatest success in the so-called gauge field theories, that provided the theoretical basis for the *Standard Model* of elementary particles (Weinberg, Salam and Glashow, and Veltman and 't Hooft), which encompasses our present knowledge of the fundamental constituents of matter. At the same time the mathematical basis of the theory is still not understood. Various approaches have been tried for developing such a basis. *Axiomatic quantum field theory* in the late nineteen fifties (Wightman) has given a beautiful set of general axioms, with important theorems proved, but with only the free fields ax examples; *Constructive field theory* (Glimm and Jaffe) have later worked on nontrivial examples, with a certain success for a limited class of simplified models. *Algebraic quantum field theory*, using C^*-algebras, with Haag and Araki as pioneers, again has lead to interesting theorems, but very little on explicit nontrivial examples. Because of all this the mathematical investigation of quantum field theory remains completely open.

6.7. References

[1]. A. Einstein
Zur Elektrodynamik bewegter Körper
Annalen der Physik 17, 891-921 (1905)

Einstein's first paper on the theory of relativity. For an English translation of this paper, see Ref.[3].

[2]. Hermann Minkowski
Raum und Zeit
Teubner Verlag 1909

This is the text of the talk Minkowski gave in 1908. He died suddenly shortly before it was published. For an English translation, see Ref.[4].

[3]. Scott Walter
Minkowski, Mathematicians, and the Mathematical Theory of Relativity
In: *The Expanding World of General Relativity*
H. Goenner, J, Renn, J. Ritter, T. Sauer (eds.)
Birkhäuser 1999

Available at :
`http://www.univ-nancy2.fr/DepPhilo/walter/papers/einstd7.pdf`

[4]. A. Einstein, H.A. Lorentz, H. Weyl, H. Minkowski
The Principle of Relativity
A collection of original papers on the special and general theory of relativity
Translated from the 1913 German edition, Dover 1952

All these pioneering papers are very readable. A treasure for the history of relativity theory.

[5]. N.M.J, Woodhouse
Special Relativity
Springer 2003

[6]. Domenico Giulini
Special Relativity: A First Encounter
Oxford University Press 2011

[7]. Wolfgang Rindler
Introduction to Special Relativity. Second edition
Oxford University Press 1991

Three books selected from the many excellent introductory books on special relativity.

[8]. P.A.M. Dirac
The Quantum Theory of the Electron
Proceedings of Royal Society London A 117, 610-624 (1928)

[9]. P.A.M. Dirac
A Theory of Electrons and Protons
Proceedings of Royal Society London A 126, 360-365 (1930)

These two papers are Dirac's greatest contribution to theoretical physics.

[10]. Sander Bais
The Equations. Icons of Knowledge
Amsterdam University Press 2011. 96 pages

A nice little book showing the beauty of the formulas of modern theoretical physics.

[11]. J.M. Cook
The Mathematics of Second Quantization
Trans. Amer. Math. Soc. 74, 222-245 (1953)

[12]. Mark Srednicki
Quantum Field Theory
Cambridge University Press 2007

Introductory.

[13]. Steven Weinberg
The Quantum Theory of Fields
I. Foundations
II. Modern Applications
III. Supersymmetry
1991-2002

The standard textbook for serious physics students.

[14]. Raymond F. Streater, Arthur S. Wightman
PCT, Spin and Statistics, and All That Princeton University Press 2000

An introduction to Wightman axiomatic field theory.

[15]. Huzihuro Araki
Mathematical Theory of Quantum Fields
Oxford University Press 2009

An excellent introduction to algebraic quantum field theory by one of its creators.

[16]. Rudolf Haag
Local Quantum Physics: Fields, Particles, Algebras
Second revised and enlarged edition
Springer 1996

More comprehensive.

[17]. P.J.M. Bongaarts *Maxwell's equations in axiomatic quantum field theory*
I. Field tensor and potentials
II. Covariant and noncovariant gauges
Journal of Mathematical Physics I: 18, 1510-1516 (1977), II: 23, 1881-1898 (1982).

Figure 1: Hermann Minkowski

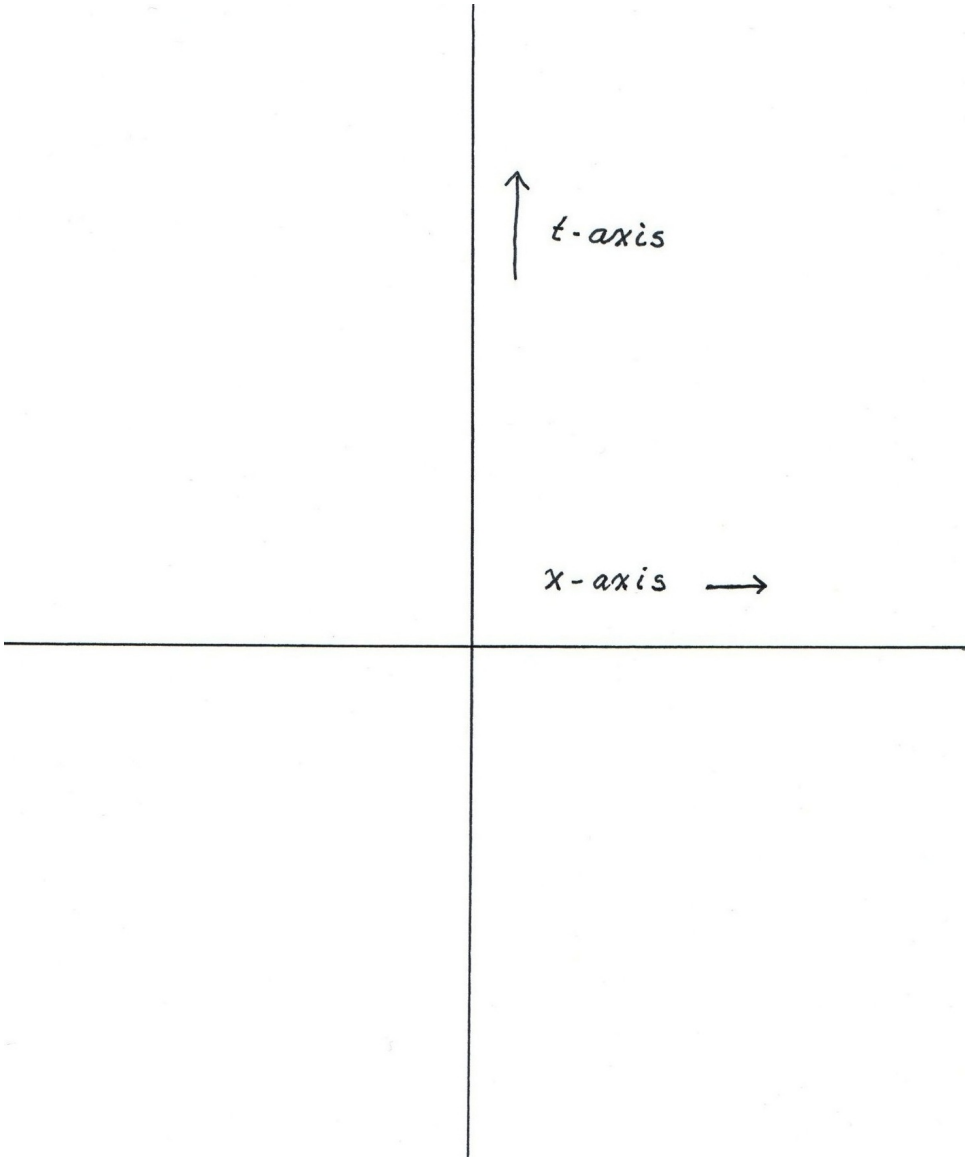

Figure 2: Empty spacetime

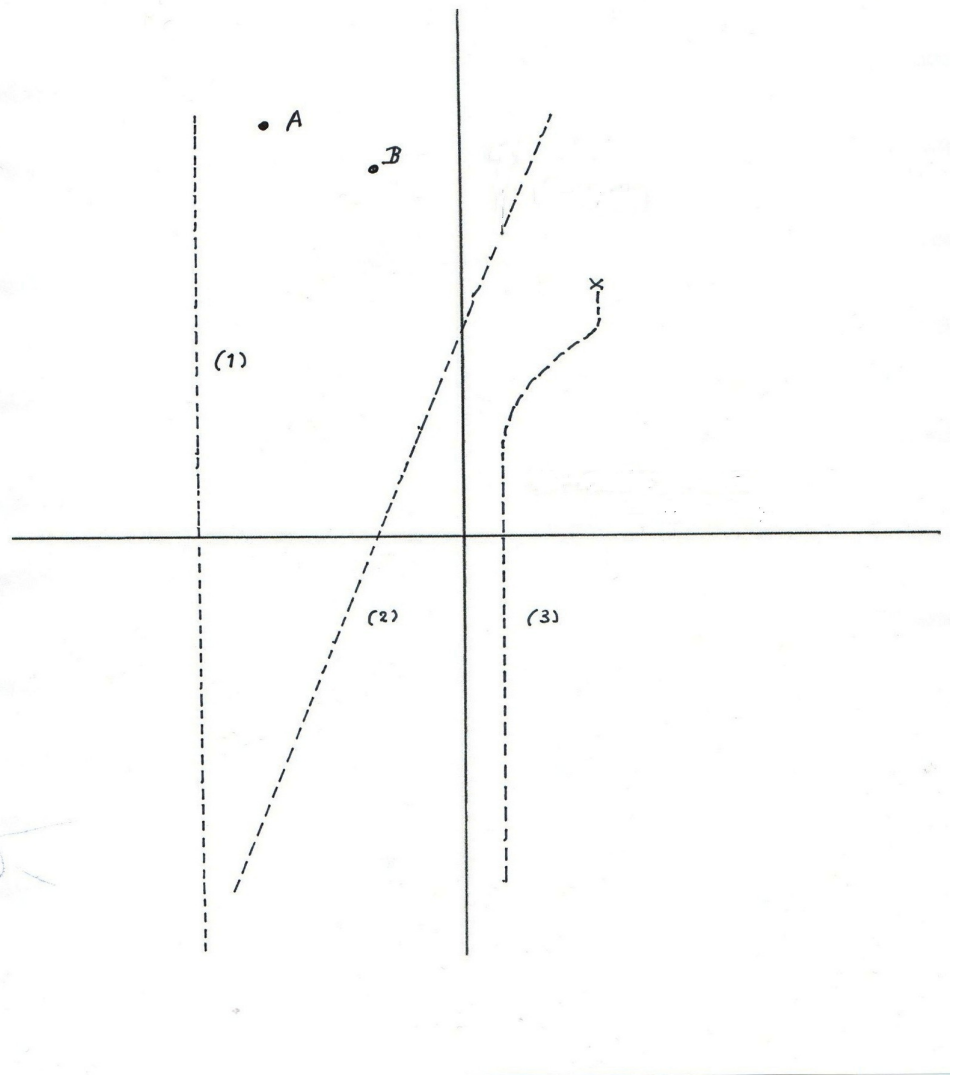

Figure 3: Events and worldlines

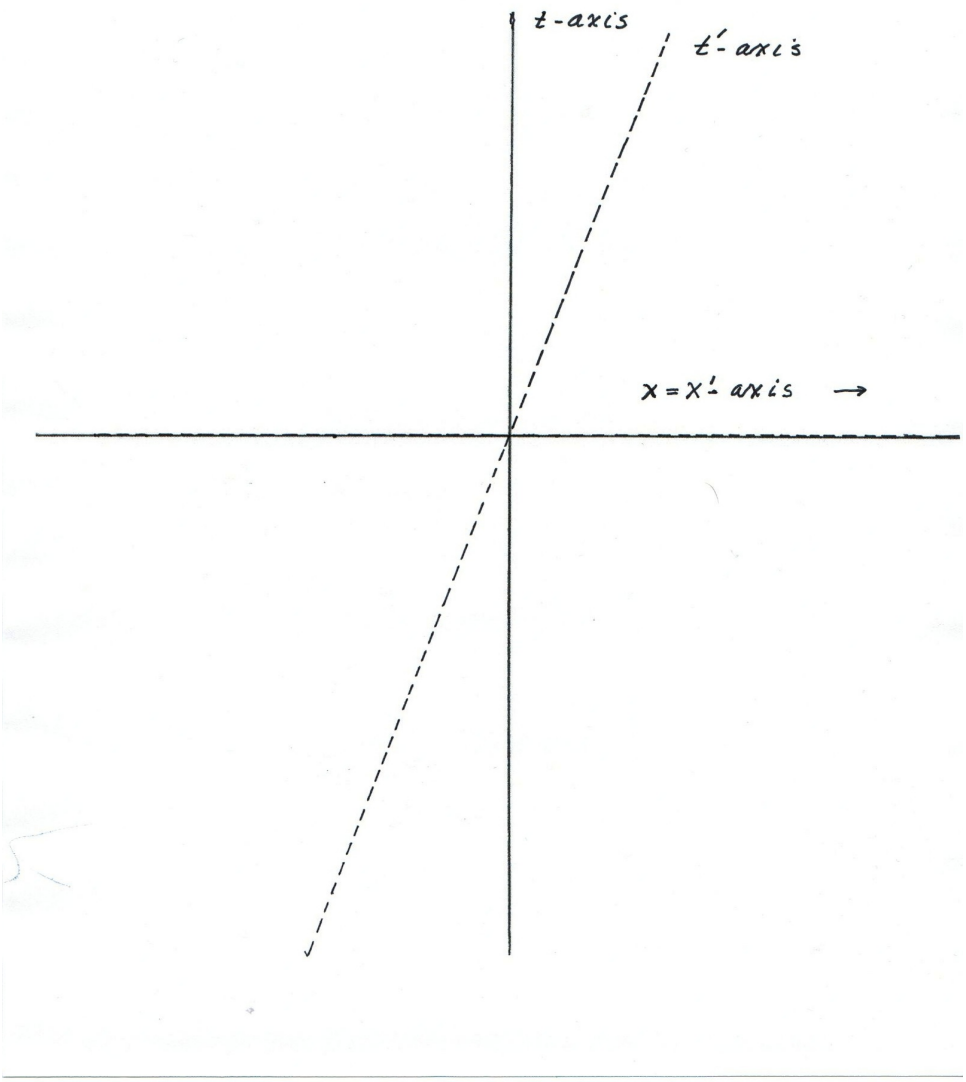

Figure 4: Galileo transformation

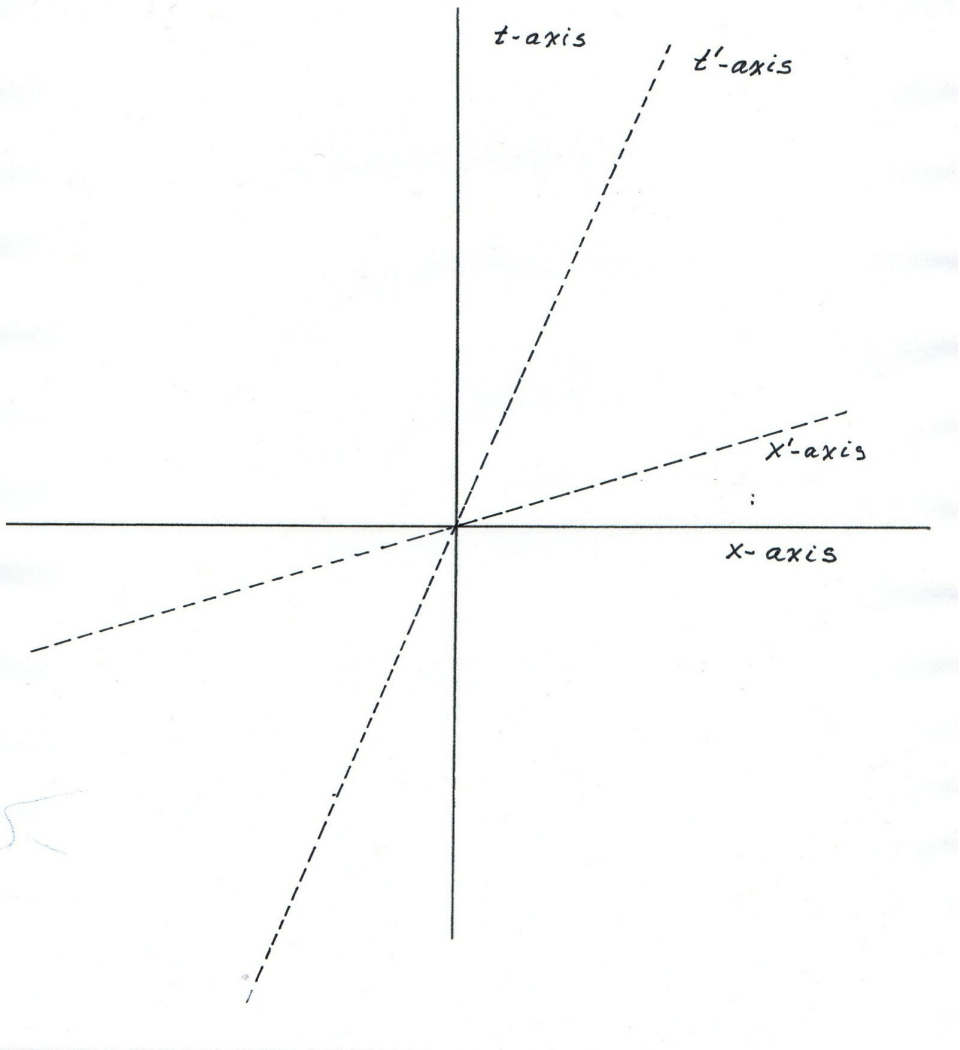

Figure 5: Lorentz transformation

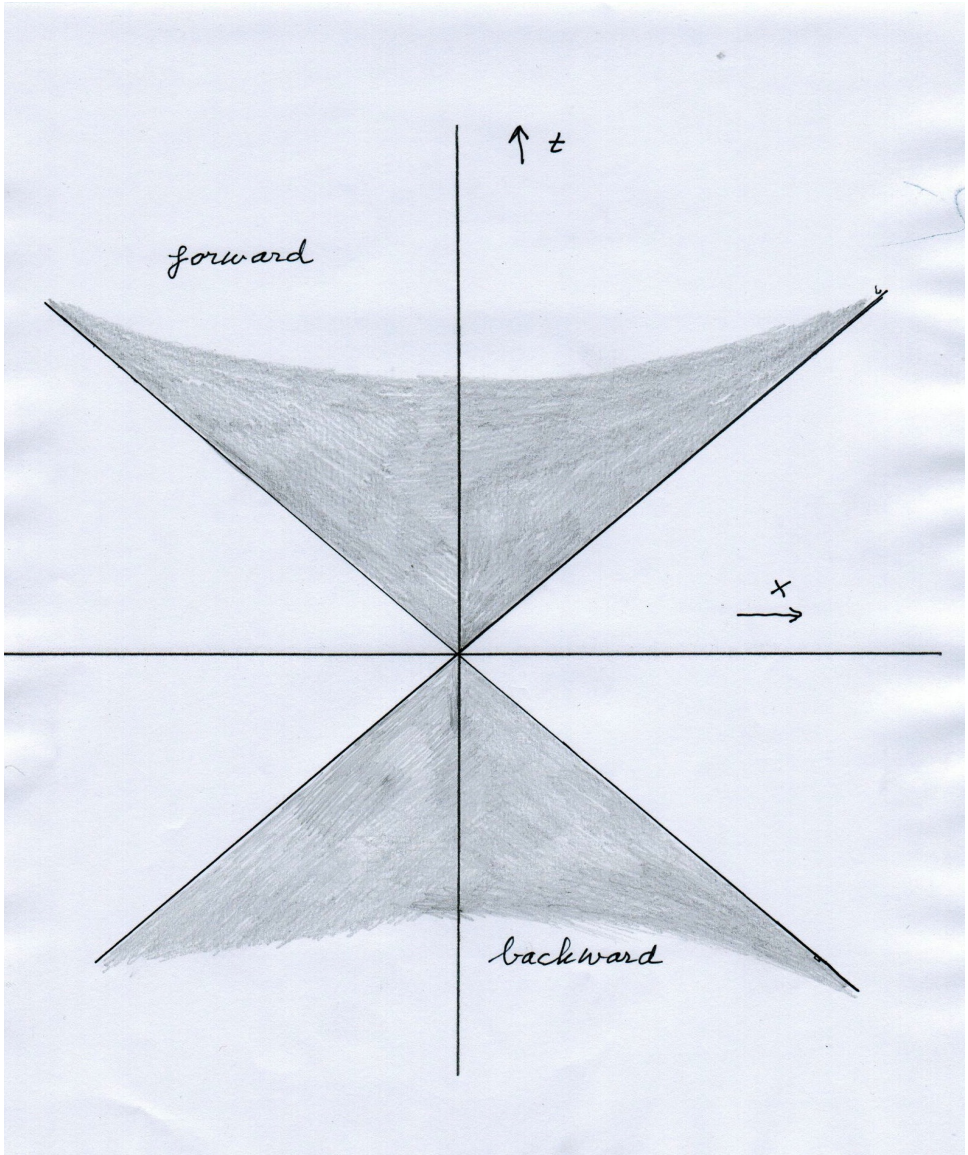

Figure 6: Light cone

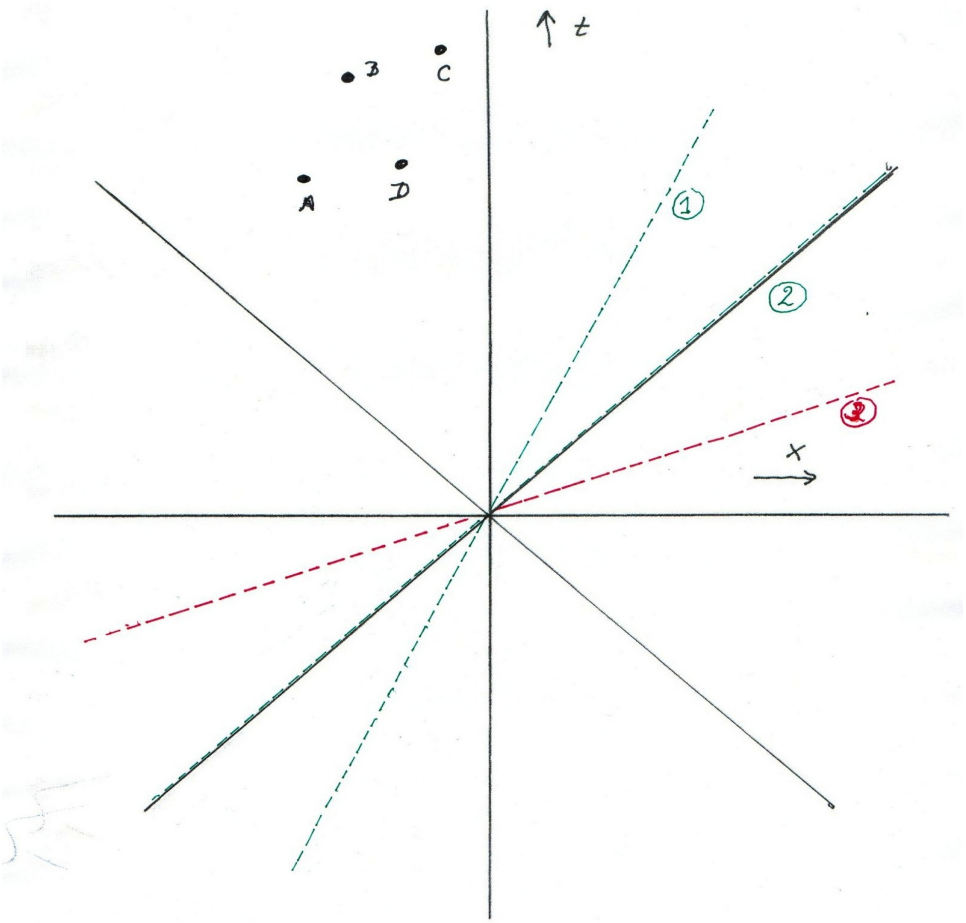

Figure 7: Events, motion with various velocities