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ÚSTAV TEORETICKÉ FYZIKY A ASTROFYZIKY

# **Bakalářská práce**

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**MILAN SUK**



# **Aspekty přechodu od kvantové mechaniky ke kvantové teorii pole**

Bakalářská práce

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# **Abstrakt**

V této bakalářské/diplomové/rigorózní práci se věnujeme ...

# **Abstract**

In this thesis we study ...



**Místo tohoto listu vložte kopii oficiálního (podepsaného) zadání práce.**



# Poděkování

Na tomto místě bych chtěl(-a) poděkovat ...

# Prohlášení

Prohlašuji, že jsem svoji bakalářskou/diplomovou/rigorózní práci vypracoval(-■  
a) samostatně s využitím informačních zdrojů, které jsou v práci citovány.

Brno 1. května 2018

.....  
Milan Suk



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# Nomenclature

- $\mathbb{C}$  množina všech komplexních čísel
- $\mathbb{R}$  množina všech reálných čísel
- $\mathbb{Z}$  množina všech celých čísel



# Introduction

The Quantum Mechanics (QM) is a fundamental theory in physics which aims to describe the world at the lowest scales of measured units. It had a great success of explaining a lot of new observations in the very beginning of 20th century, e.g. spectra of atoms, the black-body radiation or photoelectric effect. In 1905, Albert Einstein published his famous article *On the Electrodynamics of Moving Bodies* and proposed the Special theory of relativity (STR). STR corrects the classical mechanics in a way that it can predict a state of a physical system having *relativistic velocities* and setups a new restrictions for mathematical formulations of physical theories.

A logical step is to develop a physical theory which preserves STR and is capable of describing particles in quantum mechanics. This theory is known as Relativistic Quantum Mechanics (RQM) and it has been successful in prediction of interesting phenomena in physics like antimatter or spin. Nevertheless, RQM can't be introduced without formal inconsistencies and it can't deal with varying number of particles. The modern framework which consistently combines QM and STR is the Quantum Field Theory (QFT).

The thesis consists of three main chapters. In the first one we will discuss the formulation of RQM, i.e. we will construct two relativistic quantum mechanical equations - the Klein-Gordon equation and the Dirac equation. In the second chapter we will focus on the failures of these formulations and we show the need for a new theory. In the last chapter we will briefly introduce the new framework of QFT. In the terms of Quantum scalar fields we will try to check whether the new formulation solves the problems described in the second chapter.



# Chapter 1

## Relativistic quantum mechanics

In this chapter (TODO)

### 1.1 Canonical quantization

Canonical quantization is a process of transition from a classical theory to the quantum one, i.e. procedure for quantizing the theory. The term *canonical* comes from (TODO).

**Definition 1.** Given two functions  $f(\vec{q}, \vec{p}, t)$  and  $g(\vec{q}, \vec{p}, t)$ , the binary operation  $\{f, g\}$  is called the **Poisson bracket** of these functions and takes the form

$$\{f, g\} = \sum_{i=1}^N \left( \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \quad (1.1)$$

**Theorem 1.** The Poisson brackets of canonical coordinates  $q_i$  and  $p_i$  are

$$\begin{aligned} \{q_i, q_j\} &= 0 \\ \{p_i, p_j\} &= 0 \\ \{q_i, p_j\} &= \delta_{ij} \end{aligned} \quad (1.2)$$

*Proof.* The proof of 1 can be easily done from the definition 1. The first two equations are manifestly zero because  $\frac{\partial q_i}{\partial p_j} = \frac{\partial p_i}{\partial q_j} = 0$  and the last can one be proved as follows.

$$\begin{aligned} \{q_i, p_j\} &= \sum_{k=1}^N \left( \frac{\partial q_i}{\partial q_k} \frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \frac{\partial p_j}{\partial q_k} \right) = \sum_{k=1}^N \frac{\partial q_i}{\partial q_k} \frac{\partial p_j}{\partial p_k} = \begin{cases} 1 & \text{if } i = j = k \\ 0 & \text{otherwise} \end{cases} \\ &\implies \{q_i, p_j\} = \delta_{ij} \end{aligned} \quad (1.3)$$

□

Dirac has formulated a technique for generating quantum operators from classical functions. The famous statement goes as follows.

$$\{A, B\} \rightarrow \frac{1}{i\hbar}[\hat{A}, \hat{B}] \quad (1.4)$$

For the next discussion let's define  $\mathcal{O}$  map which takes a function from the configuration space and maps it to the Hilbert space.

**Definition 2.** Let  $\mathcal{Q}$  be a configuration space and  $H$  a Hilbert space.  $End(V)$  is an endomorphism of space  $V$ , i.e. a set of linear operators  $\{L : V \rightarrow V \mid L \text{ linear}\}$ .

$$\begin{aligned} \mathcal{O} : \mathcal{Q} &\rightarrow End(H) \\ \mathcal{O}(\{f, g\}) &= \frac{1}{i\hbar}[\hat{A}, \hat{B}] \end{aligned} \quad (1.5)$$

Where  $\hat{A}$  is the operator corresponding the the classical value  $f$  and  $B$  corresponds to  $g$ .

Now we will use the fact that  $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$  to show that  $\mathcal{O}(q_i) = \hat{q}_i$ . Firstly, we will rewrite  $q$  using the Poisson bracket. The obvious choice is  $q_i = \{\frac{q_i^2}{2}, p_i\}$ . And from the definition 2 we see that  $\mathcal{O}(\{\frac{q_i^2}{2}, p_i\}) = \frac{1}{i\hbar}[\frac{\hat{q}_i^2}{2}, \hat{p}_i]$ . Using the identity for commutation relation  $[AB, C] = [A, B]C + B[A, C]$ <sup>1</sup> the commutator on the right-hand side can be written as follows.

$$\mathcal{O}(x_i) = \frac{1}{i\hbar} \left[ \frac{\hat{x}_i^2}{2}, \hat{p}_i \right] = \frac{1}{2i\hbar} (\hat{x}_i[\hat{x}_i, \hat{p}_i] + [\hat{x}_i, \hat{p}_i]\hat{x}_i) = \frac{1}{2i\hbar} (\hat{x}_i i\hbar + i\hbar \hat{x}_i) = \hat{x}_i$$

The proof of  $\mathcal{O}(p) = \hat{p}$  is very similar.

$$\mathcal{O}(p_i) = \frac{1}{i\hbar} \left[ \hat{x}_i, \frac{\hat{p}_i^2}{2} \right] = \frac{1}{2i\hbar} ([\hat{x}_i, \hat{p}_i]\hat{p}_i + \hat{p}_i[\hat{x}_i, \hat{p}_i]) = \frac{1}{2i\hbar} (i\hbar\hat{p}_i + \hat{p}_i i\hbar) = \hat{p}_i$$

In the  $x$ -representation the explicit form of  $\hat{x}$  and  $\hat{p}$  is  $\hat{x} = x$  and  $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ .  
TODO: study  $\mathcal{O}(\{f(\vec{q}, \vec{p})\})$  and  $\mathcal{O}(\{f + g, h\})$ . How to get  $\mathcal{O}(E)$ ?

## 1.2 Klein-Gordon equation

*Klein-Gordon equation* is relativistic quantum mechanical equation named after Oskar Klein and Walter Gordon and it describes relativistic spinless particles. It can be found using quantization of the relativistic energy equation. We need to apply the  $\mathcal{O}$  map on each side while taking into account that  $\mathcal{O}(E^2) = -\hbar^2\frac{\partial^2}{\partial t^2}$  and  $\mathcal{O}(\vec{p}^2) = -\hbar^2\Delta$ .

<sup>1</sup>Proof by directly using the definition of the commutator:  $[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B, C] + [A, C]B$

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

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = -\hbar^2 c^2 \Delta \psi + m^2 c^4 \psi$$

After a little rearranging and setting  $\frac{m^2 c^2}{\hbar^2} = \mu^2$ , we will finally get the famous form 1.6.

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta + \mu^2 \right) \psi = 0 \quad (1.6)$$

Let's rewrite the equation in a form so we can see it is *lorentz invariant*. We use the fact that *4-gradient* transforms the same way as any other 4-vector and then express the Klein-Gordon equation using 4-gradient dot products. Using the metric  $\eta^{\mu\nu} = \text{diag}(1, -1, -1, -1)$  and the *4-gradient*  $\partial_\mu = (\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$  it is possible to write the term  $\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta$  as follows.

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} = \eta^{\mu\nu} \partial_\mu \partial_\nu = \partial_\nu \partial^\nu$$

$$\left( \partial_\nu \partial^\nu + \mu^2 \right) \psi = 0 \quad (1.7)$$

### 1.3 Dirac equation

One important fact about the Klein-Gordon equation is that it is second-order in time. Thus we need one more initial condition compared to the Schrodinger Equation. Dirac tried to find an equation that is first order in both space and time by finding the *square root* of the Klein-Gordon equation. Let's start with the equation 1.6.

$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta + \mu^2 \right) \psi = 0$$





# Chapter 2

## Failures of the Relativistic Quantum Mechanics

In this chapter we will discuss the problems of relativistic quantum mechanics. We will start with the problem of probability density within the Klein-Gordon equation.

### 2.1 Probability density

In the non-relativistic case we can find the continuity equation by taking the complex conjugate of the Schrodinger's equation.

$$\begin{aligned}i\hbar \frac{\partial}{\partial t} \psi &= \hat{H} \psi \\ -i\hbar \frac{\partial}{\partial t} \psi^* &= (\hat{H} \psi)^*\end{aligned}$$

Then we multiply the first equation by  $\psi^*$  and the second one by  $\psi$ .

$$\begin{aligned}i\hbar \psi^* \frac{\partial}{\partial t} \psi &= \psi^* \hat{H} \psi \\ i\hbar \psi \frac{\partial}{\partial t} \psi^* &= \psi (\hat{H} \psi)^*\end{aligned}$$

If we subtract these two equations from each other and use the formula for derivative  $(a \cdot b)' = a' \cdot b + a \cdot b'$  we will get a form from which it will be easy to identify the continuity equation  $\frac{\partial \rho}{\partial t} + \text{div} \vec{j} = 0$ .

$$i\hbar \frac{\partial |\psi|^2}{\partial t} = \psi^* \hat{H} \psi - \psi (\hat{H} \psi)^*$$

We assume the potential  $V$  in  $\hat{H} = \frac{\hat{p}^2}{2m} + V$  to be real-valued thus the right-hand side will simplify to

$$\psi^* \frac{\hbar^2}{2m} \nabla^2 \psi - \psi \frac{\hbar^2}{2m} \nabla^2 \psi^* = \frac{\hbar^2}{2m} \left( \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right)$$

and the desired form is

$$\frac{\partial |\psi|^2}{\partial t} + \text{div} \left[ \frac{\hbar}{2mi} \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right) \right] = 0$$

Now we will do the same for the Klein-Gordon equation 1.6. Let's do the same procedure here and find the complex conjugate, multiply both equations by  $\psi$  and  $\psi^*$  and then subtract them. After that let's focus on the term which contains the time derivative and thus will represent the *probability density*.

$$\frac{\partial \rho}{\partial t} \sim \frac{1}{2i} \left[ \psi^* \frac{\partial^2}{\partial t^2} \psi - \psi \frac{\partial^2}{\partial t^2} \psi^* \right]$$

Now we can find what  $\rho$  is proportional to.

$$\rho \sim \frac{1}{2i} \left[ \psi^* \frac{\partial}{\partial t} \psi - \psi \frac{\partial}{\partial t} \psi^* \right] \quad (2.1)$$

Let's divide the wave function  $\psi$  into the real and imaginary part.

$$\begin{aligned} \psi &= i\psi_1 + \psi_2 \\ \rho &\sim \left[ \psi_2 \frac{\partial}{\partial t} \psi_1 - \psi_1 \frac{\partial}{\partial t} \psi_2 \right] \end{aligned}$$

Now it is easy to see the problem. In the non-relativistic case the probability density was simply  $|\psi|^2$  which is non-negative for any  $\psi : \mathbb{R} \rightarrow \mathbb{C}$ . In the case of Klein-Gordon equation, we can see the probability density is zero whenever the wave function is either exclusively real or imaginary. Moreover, since both  $\frac{\partial \psi_1}{\partial t}$  and  $\frac{\partial \psi_2}{\partial t}$  are arbitrary, the value can be negative. This is in contradiction with the interpretation of  $\rho$  as the *probability density of measuring the system within a given state  $\psi$* .

## 2.2 Causality

Now we would like to investigate the problem of causality in the quantum mechanics. We're going to study the transition amplitude of a free particle to propagate from one space-time point to another one. We will assume the standard definition of the causality in physics.

**Definition 3.** Suppose we understand what is meant by a cause  $C$  and a effect  $E$ . If  $C$  happens before  $E$  and  $E$  is in the future lightcone from the perspective of  $C$  then there might be a causality between  $C$  and  $E$ . Or formulated more usefully for the computation - if  $X_C = (0, 0)$  is the  $C$ 's space-time event and  $X_E = (x_E, ct_E)$  is the  $E$ 's space-time event then  $X_C$  can cause the  $X_E$  if  $t_E > |x_E|$ .

We will follow the same calculation like in [3]. In the correspondence with the fact that the space translation is generated by the momentum operator  $\hat{p}$ , the time evaluation is generated by the energy operator  $\hat{H}$ . So if we know

the state of the system  $|x_0\rangle = |x(t=0)\rangle$ , the state in the future will be  $|x_0\rangle = |x(t=t')\rangle = \hat{U}(0, t') |x_1\rangle = \exp\left\{-\frac{i}{\hbar} \hat{H} t'\right\} |x_0\rangle$ . The amplitude of the system going from the state  $|x_0\rangle$  to  $|x_1\rangle$  is

$$\langle x_1 | \exp\left\{-\frac{i}{\hbar} \hat{H} t'\right\} | x_0 \rangle \quad (2.2)$$

which we will evaluate using the identity  $\hat{I}$  expressed in the continuous basis  $\{|p\rangle\}$  and the expression for  $\langle p|x\rangle = \exp\left\{-\frac{i}{\hbar} p x\right\}$ . We will assume a single particle without an external potential thus the Hamiltonian is simply  $\hat{H} = \frac{\hat{p}^2}{2m}$ .

$$\begin{aligned} A_1 &= \langle x_1 | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} t'} | x_0 \rangle = \int dp \langle x_1 | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} t'} | p \rangle \langle p | x_0 \rangle = \\ &= \int dp e^{-\frac{i}{\hbar} \frac{p^2}{2m} t'} \langle x_1 | p \rangle \langle p | x_0 \rangle = \int dp e^{-\frac{i}{\hbar} \frac{p^2}{2m} t'} e^{\frac{i}{\hbar} p(x_1 - x_0)} = \\ &= \int dp e^{-\frac{i}{\hbar} \left[ \frac{p^2}{2m} t' - p(x_1 - x_0) \right]} = \left| \frac{t'}{2m} \left[ p - \frac{m}{t'}(x_1 - x_0) \right]^2 - \frac{m}{2t'}(x_1 - x_0)^2 \right| = \\ &= e^{\frac{im}{2\hbar t'}(x_1 - x_0)^2} \int dp e^{-\frac{it'}{2\hbar m} \left[ p - \frac{m}{t'}(x_1 - x_0) \right]^2} \end{aligned}$$

In the integral we can substitute  $p \rightarrow p + -\frac{m}{t'}(x_1 - x_0)$  without the change of boundaries. TODO imaginary gaussian integral

$$A_1 = \sqrt{\frac{2\hbar m \pi}{it'}} e^{\frac{im}{2\hbar t'}(x_1 - x_0)^2} \quad (2.3)$$

From the final result 2.3 we see that the probability of measuring the transition  $(x_0, 0) \rightarrow (x_1, t')$  will be

$$P_1 \sim \frac{1}{t'}$$

thus for an arbitrary choice of  $(x_1 - x_0)$  there is no fixed time  $t'$ . This results in a possibility for the particle being outside of the lightcone with a non-zero probability. This result clearly violates the causality. But the conclusion is not unexpected in the case of the non-relativistic free particle. We used the definition within the relativity theory to formulate the condition for the causality but the Hamiltonian  $\hat{H}$  doesn't even include the  $c$  constant. We could try to get a proper result by assuming the relativistic energy 2.4. As we have shown, a quantization of such an expression lead us to the Klein-Gordon equation which has the Lorentz symmetry and thus is a good candidate for the right transition amplitude.

$$E^2 = \vec{p}^2 c^2 + m^2 c^4 \quad (2.4)$$

The hamiltonian for such a case is  $\hat{H} = c\sqrt{\hat{p}^2 + (mc)^2}$ . The new amplitude  $A_2$  is then given by

$$\begin{aligned}
A_2 &= \langle x_1 | e^{-\frac{i}{\hbar} c \sqrt{\hat{p}^2 + (mc)^2} t'} | x_0 \rangle = \int dp \langle x_1 | e^{-\frac{i}{\hbar} c \sqrt{p^2 + (mc)^2} t'} | p \rangle \langle p | x_0 \rangle = \\
&= \int dp e^{-\frac{i}{\hbar} c \sqrt{p^2 + (mc)^2} t'} e^{\frac{i}{\hbar} p(x_1 - x_0)}
\end{aligned}$$

# **Chapter 3**

## **Quantum field theory**

### **3.1 Scalar field**

In non-relativistic case we can find the continuity equation by

### **3.2 Second quantization**

### **3.3 Causality problem**



# Conclusion





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