MASARYKOVA UNIVERZITA PŘÍRODOVĚDECKÁ FAKULTA ŮSTAV TEORETICKÉ FYZIKY A ASTROFYZIKY

Bakalářská práce

BRNO 2018

MILAN SUK



ŮSTAV TEORETICKÉ FYZIKY A ASTROFYZIKY

Aspekty přechodu od kvantové mechaniky ke kvantové teorii pole

Bakalářská práce

Milan Suk

Vedoucí práce: doc. Klaus Bering Larsen, Ph.D Brno 2018

Bibliografický záznam

Autor: Milan Suk

Přírodovědecká fakulta, Masarykova univerzita

Ůstav teoretické fyziky a astrofyziky

Název práce: Aspekty přechodu od kvantové mechaniky ke kvan-

tové teorii pole

Studijní program: Fyzika

Studijní obor: Fyzika

Vedoucí práce: doc. Klaus Bering Larsen, Ph.D

Akademický rok: 2017/2018

Počet stran: ?? + ??

Klíčová slova: kvantová mechanika, kvantová teorie pole, relativi-

stická kvantová mechanika

Bibliographic Entry

Author: Milan Suk

Faculty of Science, Masaryk University Department of physics and astrophysics

Title of Thesis: Aspects of the transition from quantum mechanics

to quantum field theory

Degree Programme: Physics

Field of Study: Physics

Supervisor: doc. Klaus Bering Larsen, Ph.D

Academic Year: 2017/2018

Number of Pages: ?? + ??

Keywords: quantum mechanics; quantum field theory, rela-

tivistic quantum mechanics

Abstrakt

 \mathbf{V} této bakalářské/diplomové/rigorózní práci se věnujeme ...

Abstract

In this thesis we study \dots



Poděkování

Na	tomto	místě	hych	chtěl(-a)) poděkovat
ıva.	COLLICO	mste	DVCII	circen-a.	, bouekovat

Prohlášení

Prohlašuji, že jsem svoji bakalářskou/diplomovou/rigorózní práci vypra a) samostatně s využitím informačních zdrojů, které jsou v práci citován				
D 1 1 Ye 9010				
Brno 1. května 2018	Milan Suk			

Contents

Nomenclature	XV
Introduction	1
Kapitola 1 lativistic quantum mechanics	3
1.1 Canonical quantization	3
1.2 Klein-Gordon equation	5
1.3 Dirac equation	6
Kapitola 2 ilures of the Relativistic Quantum Mechanics	7
2.1 Probability density	7
2.2 Ground state	10
2.3 Causality	10
Kapitola 3 antum field theory	15
3.1 Scalar field	15
3.2 Second quantization	15
3.3 Causality problem	15
Conclusion	17
Bibliography	19

Nomenclature

- $\mathbb C \quad$ 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 cant 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 eqautions - 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 we will introduce the basics of the canonical quantization. We will start by introducing the Poisson brackets and it's basic properties. Then we will define a quantization map \mathcal{O} which maps the classical dynamical variable into the operator within a Hilbert space. Using this process we will then formulate the Klein-Gordon equation, an equation for describing a spinless particle in the quantum mechanics. We will see that this equation is second order both in time and space which will result some obstacles. With the hope of solving this issue we will construct the Dirac equation which describes the $\frac{1}{2}$ -spin particle.

1.1 Canonical quantization

Canonical quantization is a process of transition from a classical theory to the quantum one. If a quantum problem has an analog in the classical mechanics we can use the process of quantization to find the formulation in the quantum mechanics using the analogous equations in the classical one. In the classical mechanics a state of the system is represented by coordinates in the *phase space* $(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n}, t)$. In the quantum mechanics, the analog of q_i and p_i are operators $\hat{q_i}$ and $\hat{p_i}$ acting in the *Hilbert space*.

Definition 1. Given two dynamical variables in the phace space \mathcal{Q} , $f(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n}, t) \in C^{\infty}(\mathcal{Q}, \mathcal{R})$ and $g(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n}, t) \in C^{\infty}(\mathcal{Q}, \mathcal{R})$, the binary operation $\{f, g\}$ is called the **Poisson bracket** of these functions and takes the form

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

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

$$\{q_i, q_j\} = 0$$

 $\{p_i, p_j\} = 0$
 $\{q_i, p_j\} = \delta_{ij}$ (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 one can be proved as follows.

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

$$\implies \{q_i, p_j\} = \delta_{ij}$$

$$(1.3)$$

Paul Dirac has formulated a technique for generating operators in H from dynamical variables in $C^{\infty}(\mathcal{Q}, \mathcal{R})$. The famous statement goes as follows.

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

That means that if we have dynamical variables A and B we can get their quantum conterparts \hat{A} and \hat{B} and the defining property is the equation 1.4. Let's define the properties of the \mathcal{O} map (see [7]) and then study some consequences.

Definition 2. Let Q be a configuration space and H the corresponding Hilbert space. The quantization map is

$$\mathcal{O}: C^{\infty}(\mathcal{Q}, \mathcal{R}) \to Op(H)$$
 (1.5)

having the properties:

- 1. O is linear,
- 2. $\mathcal{O}(f)$ is self-adjoint, $f \in C^{\infty}(\mathcal{Q}, \mathcal{R})$,
- 3. the relation between commutator and the Poisson bracket is

$$\mathcal{O}(\{A,B\}) = \frac{1}{i\hbar}[\hat{A},\hat{B}] \tag{1.6}$$

- 4. a complete set $\{f_1, \ldots, f_n\}$ is mapped to a complete set $\{\mathcal{O}(f_1), \ldots, \mathcal{O}(f_n)\}$,
- 5. an identity $Id_{\mathcal{Q}}$ is mapped to the indentity $Id_{\mathcal{H}} = \mathcal{O}(Id_{\mathcal{Q}})$

It is convinient to use $[\hat{q}_i,\hat{p}_j]=i\hbar\delta_{ij}$ and 1.6 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 1.6 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 $[AB,C]=[A,B]C+B[A,C]^1$ the commutator on the right-hand side can be written as follows.

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

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

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

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

TODO: Groenewold theorem, Deformation quantization and geometric quantization note.

From now, we will use the explicit form of the operators in the *x-representation*.

$$\mathcal{O}(p_i) = -i\hbar \frac{\partial}{\partial x^i}$$

$$\mathcal{O}(E) = i\hbar \frac{\partial}{\partial t}$$
(1.7)

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 $\mathcal{O}(\vec{p}^2) = -\hbar^2 \Delta$.

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

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

After a little rearranging and setting $\frac{m^2c^2}{\hbar^2} = \mu^2$, we will finally get the famous form 1.8.

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \mu^2\right)\psi = 0 \tag{1.8}$$

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 than express the Klein-Gordon equation using 4-gradient dot products. Using the metric $\eta^{\mu\nu}=diag(1,-1,-1,-1)$ 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.

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} = \eta^{\mu\nu} \partial_{\mu} \partial_{\nu} = \partial_{\nu} \partial^{\nu}
\left(\partial_{\nu} \partial^{\nu} + \mu^2 \right) \psi = 0$$
(1.9)

1.3 Dirac 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 1.8.

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

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. We will show that the probability density is positive-definite for Dirac Equation but is not in the of the Klein-Gordon equation. Then we will

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.

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

Then we mutiply the first equation by ψ and the second one by ψ^* .

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

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

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

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

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

Now we will do the same for the Klein-Gordon equation 1.8. Let's do the same procedure here and find the complex conjugate, multiply both equations by ψ and ψ^* and then substract them. After that let's focus on the term which contains the time derivative a 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 ρ is proportial to.

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

Let's divide the wave function ψ into the real and imaginary part.

$$\psi = i\psi_1 + \psi_2$$

$$\rho \sim \left[\psi_2 \frac{\partial}{\partial t} \psi_1 - \psi_1 \frac{\partial}{\partial t} \psi_2 \right]$$

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 $\psi:\mathbb{R}\to\mathbb{C}$. 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 interretation of ρ as the *probability density of measuring the system within a given state* ψ . To solve this problem, Dirac introduced his equation. Let's check the probability density using the procedure of deriving the continuity equation from the Dirac equation [4]. Let's start with the Dirac equation of the form as follows.

$$(i\hbar\gamma^{\mu}\partial_{\mu} - mc)\psi = 0 \tag{2.2}$$

For further discussion let's introduce some useful theorems.

Theorem 2. Let γ^{μ} 's be Dirac matrices [5] defined by the properties (see [6])

$$\left\{\gamma^{\mu}, \gamma^{\nu}\right\} = 2\eta^{\mu\nu} I_4 \tag{2.3}$$

where $\eta^{\mu\nu} = diag\{+1, -1, -1, -1\}$, and

$$\left(\gamma^{\mu}\right)^{\dagger} = \gamma^{0} \gamma^{\mu} \gamma^{0} \tag{2.4}$$

then following equations hold for $\mu \in \{0, 1, 2, 3\}$, $i \in \{1, 2, 3\}$.

$$\gamma^0 \gamma^i = -\gamma^i \gamma^0 \tag{2.5}$$

$$(\gamma^0)^{\dagger} = \gamma^0$$

$$(\gamma^i)^{\dagger} = -\gamma^i$$
(2.6)

Proof. The proof of 2.5 is a direct application of the definition 2.3.

$$\{\gamma^0, \gamma^i\} = \gamma^0 \gamma^i + \gamma^0 \gamma^i = 2\eta^{0i} I_4$$
$$\gamma^0 \gamma^i + \gamma^0 \gamma^i = 0$$
$$\gamma^0 \gamma^i = -\gamma^0 \gamma^i$$

To proof 2.6 we just need to know that $\gamma^0 \gamma^0 = I_4$ which can be shown to be true because we constructed the matrices to be so or by checking the definition 2.3: $\{\gamma^0, \gamma^0\} = 2\gamma^0 \gamma^0 = 2\eta^{00}I_4$. Then we use the defining property 2.4 and the equation 2.5.

$$(\gamma^0)^{\dagger} = \gamma^0 \gamma^0 \gamma^0 = \gamma^0 I_4 = \gamma^0$$
$$(\gamma^i)^{\dagger} = \gamma^0 \gamma^i \gamma^0 = -\gamma^0 \gamma^0 \gamma^i = -I_4 \gamma^i = -\gamma^i$$

We will use a similar trick we used within the Schrodinger equation or the Klein-Gordon equation. We take the Hermitian adjoint of the left-hand side of the Dirac equation 2.2.

$$\begin{aligned} \left[i\hbar\gamma^{\mu}\partial_{\mu}\psi - mc\psi\right]^{\dagger} &= \\ &= \left[i\hbar\gamma^{0}\partial_{0}\psi + \gamma^{1}\partial_{1}\psi + \gamma^{2}\partial_{2}\psi + \gamma^{3}\partial_{3}\psi - mc\psi\right]^{\dagger} &= \\ &= -i\hbar\left[\left(\gamma^{0}\partial_{0}\psi\right)^{\dagger} + \left(\gamma^{1}\partial_{1}\psi\right)^{\dagger} + \left(\gamma^{2}\partial_{2}\psi\right)^{\dagger} + \left(\gamma^{3}\partial_{3}\psi\right)^{\dagger}\right] - mc\psi^{\dagger} &= \\ &= -i\hbar\left[\partial_{0}\psi^{\dagger}(\gamma^{0})^{\dagger} + \partial_{1}\psi^{\dagger}(\gamma^{1})^{\dagger} + \partial_{2}\psi^{\dagger}(\gamma^{2})^{\dagger} + \partial_{3}\psi^{\dagger}(\gamma^{3})^{\dagger}\right] - mc\psi^{\dagger} \end{aligned}$$

By using the equation 2.6 we evaluate all the gamma matrices with a dagger.

$$-i\hbar \left[\partial_0 \psi^{\dagger} \gamma^0 + \partial_1 \psi^{\dagger} (-\gamma^1) + \partial_2 \psi^{\dagger} (-\gamma^2) + \partial_3 \psi^{\dagger} (-\gamma^3)\right] - mc\psi^{\dagger} = 0$$
 (2.7)

Now, the trick is to introduce $\overline{\psi}:=\psi^\dagger\gamma^0$, multiply the equation 2.7 by γ^0 from the right and then rewrite all the $\psi^\dagger\gamma^0$ terms with $\overline{\psi}$ using the equation 2.5.

$$-i\hbar \left[\partial_0 \psi^{\dagger} \gamma^0 \gamma^0 + \partial_1 \psi^{\dagger} (-\gamma^1 \gamma^0) + \partial_2 \psi^{\dagger} (-\gamma^2 \gamma^0) + \partial_3 \psi^{\dagger} (-\gamma^3 \gamma^0)\right] - mc\psi^{\dagger} \gamma^0 = 0$$

$$-i\hbar \left[\partial_0 \psi^{\dagger} \gamma^0 \gamma^0 + \partial_1 \psi^{\dagger} (\gamma^0 \gamma^1) + \partial_2 \psi^{\dagger} (\gamma^0 \gamma^2) + \partial_3 \psi^{\dagger} (\gamma^0 \gamma^2)\right] - mc\psi^{\dagger} \gamma^0 = 0$$

$$-i\hbar \left[\partial_0 \overline{\psi} \gamma^0 + \partial_1 \overline{\psi} \gamma^1 + \partial_2 \overline{\psi} \gamma^2 + \partial_3 \overline{\psi} \gamma^2\right] - mc\overline{\psi} = 0$$

And finally, we will multiply this equation by ψ from the left.

$$i\hbar\partial_{\mu}\overline{\psi}\gamma^{\mu}\psi + mc\overline{\psi}\psi = 0 \tag{2.8}$$

To get rid of the $mc\overline{\psi}\psi$ term, let's take the original equation 2.2 and multiply it by $\overline{\psi}$ from the right. Then we will simply add these two equations

$$i\hbar\partial_{\mu}\overline{\psi}\gamma^{\mu}\psi + mc\overline{\psi}\psi = 0 \wedge i\hbar\overline{\psi}\gamma^{\mu}\partial_{\mu}\psi - mc\overline{\psi}\psi = 0 \implies$$

$$\partial_{\mu}\overline{\psi}\gamma^{\mu}\psi + \overline{\psi}\gamma^{\mu}\partial_{\mu}\psi = 0$$

$$\partial_{\mu}(\overline{\psi}\gamma^{\mu}\psi) = 0 \qquad (2.9)$$

From the continuity equation 2.9 we see that the probability density should be $\rho = \overline{\psi} \gamma^0 \psi$. Which is

$$\rho = \overline{\psi}\gamma^0\psi = \psi^{\dagger}\gamma^0\gamma^0\psi = \psi^{\dagger}\psi$$

and thus always a positive quantity! TODO: discussion on the results.

2.2 Ground state

2.3 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 causility in physics. TODO: discussion on the causality definition.

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 usefuly 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

$$\langle x_1 | \exp \left\{ -\frac{i}{\hbar} \hat{H} t' \right\} | x_0 \rangle$$
 (2.10)

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

$$A_{1} = \langle x_{1} | e^{-\frac{i}{\hbar} \frac{\hat{p}^{2}}{2m} t'} | x_{0} \rangle = \int dp \ \langle x_{1} | e^{-\frac{i}{\hbar} \frac{\hat{p}^{2}}{2m} t'} | p \rangle \langle p | x_{0} \rangle =$$

$$= \int dp \ e^{-\frac{i}{\hbar} \frac{p^{2}}{2m} t'} \langle x_{1} | p \rangle \langle p | x_{0} \rangle = \int dp \ e^{-\frac{i}{\hbar} \frac{p^{2}}{2m} t'} e^{\frac{i}{\hbar} p(x_{1} - x_{0})} =$$

$$= \int dp \ e^{-\frac{i}{\hbar} \left[\frac{p^{2}}{2m} t' - p(x_{1} - x_{0}) \right]} = \begin{vmatrix} \left[\frac{p^{2}}{2m} t' - p(x_{1} - x_{0}) \right] = \\ \frac{t'}{2m} \left[p - \frac{m}{t'} (x_{1} - x_{0}) \right]^{2} - \frac{m}{2t'} (x_{1} - x_{0})^{2} \end{vmatrix} =$$

$$= e^{\frac{im}{2\hbar t'} (x_{1} - x_{0})^{2}} \int dp \ e^{-\frac{it'}{2\hbar m} \left[p - \frac{m}{t'} (x_{1} - x_{0}) \right]^{2}}$$

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

$$A_1 = \sqrt{\frac{2\hbar m\pi}{it'}} e^{\frac{im}{2\hbar t'}(x_1 - x_0)^2}$$
 (2.11)

From the final result 2.11 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 conslusion 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 event include the c constant. We could try to get a proper result by assuming the relativistic energy 2.12. As we have shown, a quantization of such an expression lead us to the Klein-Gordon equation which has the Lorentz symmetry a thus is a good candidate for the right transition amplitude.

$$E^2 = \vec{p}^2 c^2 + m^2 c^4 \tag{2.12}$$

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

$$A_{2} = \langle x_{1} | e^{-\frac{i}{\hbar}c\sqrt{\hat{p}^{2} + (mc)^{2}}t'} | x_{0} \rangle = \int dp \ \langle x_{1} | e^{-\frac{i}{\hbar}c\sqrt{\hat{p}^{2} + (mc)^{2}}t'} | p \rangle \langle p | x_{0} \rangle =$$

$$= \int dp \ e^{-\frac{i}{\hbar}c\sqrt{\hat{p}^{2} + (mc)^{2}}t'} e^{\frac{i}{\hbar}p(x_{1} - x_{0})}$$

One way to analyze this integral to cheat a little bit and evaluating it using a computer numerically. To do that let's split the function inside of the integral into a real and an imaginary part.

$$\int dp \ e^{-\frac{i}{\hbar}c\sqrt{p^2 + (mc)^2}t'} e^{\frac{i}{\hbar}p(x_1 - x_0)} =$$

$$= \begin{vmatrix} k_{t'}(p) = -\frac{1}{\hbar}c\sqrt{p^2 + (mc)^2}t' \\ l_{x_1}(p) = \frac{1}{\hbar}p(x_1 - x_0) \end{vmatrix} =$$

$$= \int dp \left[\sin(k_{t'}(p))\sin(l_{x_1}(p)) - \sin(k_{t'}(p))\sin(l_{x_1}(p)) + i(\sin(k_{t'}(p))\cos(l_{x_1}(p)) + \cos(k_{t'}(p))\sin(l_{x_1}(p))) \right]$$

Now, we can integrate the function numerically using the Python¹ program 1 because we integrate the real part and the imaginary part separatelly. Then we can plot the final probability using the simple formula $P = |z|^2 = \sqrt{Im\{z\}^2 + Re\{z\}^2}$.

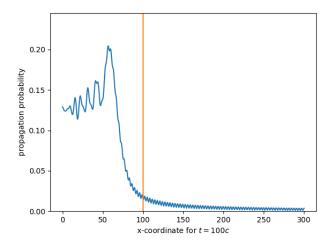


Figure 2.1: Propagation amplitude for a free relativistic particle

 $^{^1{\}rm The~script}$ uses scipy, matplotlib and numpy packages. The used interpretter was cpython, version 2.7

Listing 1: Numerical integration of the relativistic free particle propagation amplitude

```
from numpy import sqrt, cos, sin, linspace
import scipy.integrate as integrate
import matplotlib.pyplot as plt
hbar, c, m = 1, 1, 1
TIME = 100
def function(x, t):
    def real(p):
        k = -1 / hbar * c * (sqrt(p ** 2 + (m * c) ** 2)) * t
        l = 1 / hbar * p * x
        return cos(k) * cos(l) - sin(k) * sin(l)
    def imaginary(p):
        k = -1 / hbar * c * (sqrt(p ** 2 + (m * c) ** 2)) * t
        l = 1 / hbar * p * x
        return sin(k) * cos(l) + cos(k) * sin(l)
    return real, imaginary
x_list = linspace(0, 3 * TIME, 500)
y_list = []
for x in x_list:
    real, imaginary = function(x, TIME)
    r = integrate.quad(real, -c, c)
    i = integrate.quad(imaginary, -c, c)
    y_list.append(sqrt(r[0] ** 2 + i[0] ** 2) / 2)
plt.xlabel("x-coordinate for $ct = {}$".format(TIME))
plt.ylabel("propagation probability")
plt.plot(x_list, y_list)
plt.plot([TIME, TIME], [0, max(y_list) * 1.2])
plt.gca().set_ylim([0, max(y_list) * 1.2])
plt.show()
```

14

In the graph 2.1 we also plotted the vertical line which marks the point from which the event is not considered causal by our definition and the probability density should be zero there. Althought the value in the graph is reaching the zero very quickly it is very small but non-zero in the region outside of the lightcone (i.e. on the right side of the vertical marking line). So we encouter the same problem as in the calculation with the non-relativistic particle. The difference is that now we deal with an unremovable problem. We used the relativistic energy and still the theory allowed the particle to travel faster then the speed of light with non-zero probability!

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

Bibliography

- [1] S. J. Monaquel a K. M. Schmidt, On M-functions and operator theory for non-self-adjoint discrete Hamiltonian systems
- [2] Shewell, J. R. (1959). On the Formation of Quantum-Mechanical Operators. American Journal of Physics
- [3] M. Peskin and D. Schroeder, *An Introduction to Quantum Field Theory*, Westview Press, Chicago, 1995.
- [4] G. Rajasekaran, The Discovery of Dirac Equation and its Impact on Present-day Physics, 2003
- [5] Wikipedie, https://en.wikipedia.org/wiki/Gamma_matrices, 12 March 2019
- [6] Palash B. Pal, Representation-independent manipulations with Dirac matrices and spinors, Saha Institute of Nuclear Physics 1/AF Bidhan-Nagar, Calcutta 700064, INDIA
- [7] Florian Jung, Canonical group quantization and boundary conditions, Mainz Univ. (Germany). Fachbereich 08: Physik, Mathematik und Informatik