MASARYKOVA UNIVERZITA
PŘÍRODOVĚDECKÁ FAKULTA
Ústav teoretické fyziky a astrofyziky

Bakalářská práce

MILAN SUK

MASARYKOVA UNIVERZITA

Přírodovědecká fakulta
Ústav 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 2019

Bibliografický záznam

Autor: Milan Suk
                    Přírodovědecká fakulta, Masarykova univerzita
                    Ústav teoretické fyziky a astrofyziky

Název práce: Aspekty přechodu od kvantové mechaniky ke kvantové teorii pole

Studijní program: Fyzika

Studijní obor: Fyzika

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

Akademický rok: 2018/2019

Počet stran: ?? + ??

Klíčová slova: kvantová mechanika, kvantová teorie pole, relativistická kvantová mechanika

Bibliographic Entry

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 2019 ....

Milan Suk

Contents

Nomenclature

$\mathbb{C}$	complex numbers
$\mathbb{R}$	real number
$\mathcal{Q}$	configuration space which we will assume to be a simple manifold $\mathbb{R}^n$
$C^\infty(X, Y)$	Set of smooth function $f : X \to Y$
$[,]$	commutator
$\hat{H}$	Energy operator
$\hat{p}$	Momentum operator
L	Lagrangian function
$\mathcal{L}$	Lagrangian density function

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 Q 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 $\mathcal{Q}$, $f(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n}, t) \in C^\infty(\mathcal{Q}, \mathbb{R})$ and $g(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n}, t) \in C^\infty(\mathcal{Q}, \mathbb{R})$, the binary operation $\{f, g\}$ is called the **Poisson bracket** of these functions and takes the form*

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

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

$$\{q_i, q_j\} = 0$$
$$\{p_i, p_j\} = 0 \tag{1.2}$$
$$\{q_i, p_j\} = \delta_{ij}$$

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.

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

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

$\square$

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

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

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 1.9. Let's define the properties of the Q map (see [7]) and then study some consequences.

Definition 2. *Let $\mathcal{Q}$ be a configuration space and H the corresponding Hilbert space. The quantization map is*

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

having the properties:

1. Q is linear,

2. $Q(f)$ is self-adjoint, $f \in C^\infty(\mathcal{Q}, \mathbb{R})$,

3. the relation between commutator and the Poisson bracket is

$$Q(\{A, B\}) = \frac{1}{i\hbar}[\hat{A}, \hat{B}] \quad (1.6)$$

4. a complete set $\{f_1, \ldots, f_n\}$ is mapped to a complete set $\{Q(f_1), \ldots, Q(f_n)\}$,

5. an identity $Id_\mathcal{Q}$ is mapped to the indentity $Id_H = Q(Id_\mathcal{Q})$

It is convinient to use $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$ and 1.6 to show that $Q(q_i) = \hat{q}_i$. 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 $Q(\{\frac{q_i^2}{2}, p_i\}) = \frac{1}{i\hbar}[\frac{\hat{q}_i^2}{2}, \hat{p}_i]$. 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.

---

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

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

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

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

Groenewold theorem Althogh the procedure discussed so far might look promising it has a big problem. If we try to find an operator corresponding to a polynomial of q and p, $P(q, p)$, we seek a Poisson bracket $\{P_1(q, p), P_2(q, p)\} = P(p, q)$. The problem is the Poisson bracket for the $P(q, p)$ does not have to be unique. Thus we may find two different expressions $\{P_1(q, p), P_2(q, p)\}$ and $\{P_1'(q, p), P_2'(q, p)\}$ for a single $P(q, p)$ and we can end up with two different commutators $[Q(P_1), Q(P_2)] \neq [Q(P_1'), Q(P_2')]$. This reasoning was done by Groenewold to proof that the quantization postulated by 2 actually doesn't exist! The proof comes in a form of a counterexample.

Proof. Let's find a quantization of a polynomial x^2p. We can choose two different Poisson brackets, for example

$$\left\{\frac{x^3}{3}, \frac{p^2}{2}\right\} = \left((x^2p) - 0\right) = x^2p \tag{1.7}$$

$$\left\{x^2p, xp\right\} = \left((2xp)(x) - (p)(x^2))\right) = x^2p \tag{1.8}$$

now we should find the corresponding operators.

$$\left[\frac{\hat{x}^3}{3}, \frac{\hat{p}^2}{2}\right] = \frac{1}{6}\left(\hat{p}\left[\hat{x}^3, \hat{p}\right] + \left[\hat{x}^3, \hat{p}\right]\hat{p}\right) = \frac{i\hbar}{2}\left(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2\right)$$

Let's use $Q(xp) = \frac{1}{2}\left(\hat{x}\hat{p} + \hat{p}\hat{x}\right)$[2] and the very last calculation to check the result of the second expression.

$$\left[Q(\hat{x}^2\hat{p}), Q(\hat{x}\hat{p})\right] = \frac{1}{4}\left(\left[\hat{x}^2\hat{p}, \hat{x}\hat{p}\right] + \left[\hat{x}^2\hat{p}, \hat{p}\hat{x}\right] + \left[\hat{p}\hat{x}^2, \hat{x}\hat{p}\right] + \left[\hat{p}\hat{x}^2, \hat{p}\hat{x}\right]\right) =$$

$$\frac{i\hbar}{2}\left(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2 + [\hat{x}, \hat{p}]\hat{x}\right) = \frac{i\hbar}{2}\left(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2\right) - \hbar^2\hat{x}$$

Since we got two different operators for the same starting polynomial we must conclude the quantization map doesn't exist. But it's not the end of the story. As is discussed in [7] we see our results differ only by $\hbar^2$ term. Thus the quantization Q can be seen as a first order aproximation.

---

[2]Since $xp = \left\{\frac{x^2}{2}, \frac{p^2}{2}\right\}$, $Q(xp) = \left[\frac{x^2}{2}, \frac{p^2}{2}\right] = \frac{1}{4}\left(\hat{x}[\hat{x}, \hat{p}^2] + [\hat{x}, \hat{p}^2]\hat{p}\right) = \frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x})$

$$\{A, B\} \to \frac{1}{i\hbar}[\hat{A}, \hat{B}] + \mathcal{O}(\hbar^2) \tag{1.9}$$

Let's note, finally, that there is an extending procedure called *deformation quantization* which takes into account all the higher powers of $\hbar$.

$\square$

From now, we will use the explicit form of the operators in the *x-representation*.∎ As we've seen the obstruction of constructing the quantization map and we don't really want to deep dive into more complicated methods we will now use rather a heuristical approach for the 1st quantization and simply use the following quantization rules for momentem and energy.

$$\begin{aligned} p_i &\to -i\hbar\frac{\partial}{\partial x^i} \\ E &\to i\hbar\frac{\partial}{\partial t} \end{aligned} \tag{1.10}$$

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 Q map on each side while taking into account that $Q(E^2) = -\hbar^2\frac{\partial^2}{\partial t^2}$ and $Q(\vec{p}^2) = -\hbar^2\Delta$.

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

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

After a little rearranging and setting $\frac{m^2 c^2}{\hbar^2} = \mu^2$, we will finaly get the famous form 1.11.

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \mu^2\right)\psi = 0 \tag{1.11}$$

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.

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

$$\left(\partial_\mu\partial^\mu + \mu^2\right)\psi = 0 \tag{1.12}$$

1.3 Dirac equation

Dirac tried to find an equation that is first order in both space and time by doing the *square root* of the Klein-Gordon equation. Let's start with the equation 1.11.

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

We would like to find an operator $\hat{K}$ such that $\hat{K}\hat{K} = (-\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \Delta - \mu^2)$. Let's find the $\hat{K}$ in terms of coefficients γ^0, γ^1, γ^2, γ^3. If we write $\hat{K}^2 = (\hat{K}' + \mathbb{I}\mu)(\hat{K}' - \mathbb{I}\mu)$ we see it is sufficient to investigate the $\hat{K}'$ operator only since $(\hat{K}' + \mathbb{I}\mu)(\hat{K}' - \mathbb{I}\mu) = (\hat{K}')^2 - \mu^2$.

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta = (\gamma^0\frac{i}{c}\frac{\partial}{\partial t} + \gamma^1\frac{\partial}{\partial x} + \gamma^2\frac{\partial}{\partial y} + \gamma^3\frac{\partial}{\partial z})(\gamma^0\frac{i}{c}\frac{\partial}{\partial t} + \gamma^1\frac{\partial}{\partial x} + \gamma^2\frac{\partial}{\partial y} + \gamma^3\frac{\partial}{\partial z})$$

and by rewriting the expression above we get

$$(\gamma^0\frac{i}{c}\frac{\partial}{\partial t} + \gamma^1\frac{\partial}{\partial x} + \gamma^2\frac{\partial}{\partial y} + \gamma^3\frac{\partial}{\partial z})(\gamma^0\frac{i}{c}\frac{\partial}{\partial t} + \gamma^1\frac{\partial}{\partial x} + \gamma^2\frac{\partial}{\partial y} + \gamma^3\frac{\partial}{\partial z}) =$$

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}(\gamma^0)^2 + \frac{\partial^2}{\partial x^2}(\gamma^1)^2 + \frac{\partial^2}{\partial y^2}(\gamma^2)^2 + \frac{\partial^2}{\partial z^2}(\gamma^3)^2 + \frac{\partial}{\partial t}\frac{\partial}{\partial x}(\gamma^0\gamma^1 + \gamma^1\gamma^0) + \frac{\partial}{\partial t}\frac{\partial}{\partial y}(\gamma^0\gamma^2 + \gamma^2\gamma^0)\ldots$$

We see the expansion gave us the conditions for the γ's, $(\gamma^0)^2 = 1$, $(\gamma^i)^2 = -1$ and $\gamma^i\gamma^j + \gamma^j\gamma^i = 0$ for $i, j \in \{1, 2, 3\}$. To satisfy all these conditions γ^μ is clearly not a number. When Dirac was deriving the equation he immediately recognised the gammas to be 4x4 matrices.

$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

TODO: gamma matrices

The the final famous form of the Dirac equation is

$$(i\hbar\gamma^\mu\partial_\mu + mc)\psi = 0 \tag{1.13}$$

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 it is not in the case of the Klein-Gordon equation. Then we will investigate the problem of causality in the physics.

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.

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$$

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

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

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

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

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 $\frac{\partial \rho}{\partial t} + div\vec{j} = 0$.

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

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 1.11. 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.

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

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 intepretation 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 $\mu \in \{0, 1, 2, 3\}$, $i \in \{1, 2, 3\}$.

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

$$\begin{aligned} \left(\gamma^0\right)^\dagger &= \gamma^0 \\ \left(\gamma^i\right)^\dagger &= -\gamma^i \end{aligned} \tag{2.6}$$

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

$$\begin{aligned} \{\gamma^0, \gamma^i\} = \gamma^0 \gamma^i + \gamma^0 \gamma^i &= 2\eta^{0i} I_4 \\ \gamma^0 \gamma^i + \gamma^0 \gamma^i &= 0 \\ \gamma^0 \gamma^i &= -\gamma^0 \gamma^i \end{aligned}$$

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.

$$\begin{aligned} \left(\gamma^0\right)^\dagger &= \gamma^0 \gamma^0 \gamma^0 = \gamma^0 I_4 = \gamma^0 \\ \left(\gamma^i\right)^\dagger &= \gamma^0 \gamma^i \gamma^0 = -\gamma^0 \gamma^0 \gamma^i = -I_4 \gamma^i = -\gamma^i \end{aligned}$$

$\square$

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.

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

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.

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

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

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

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

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! Unfortunatelly this doesn't mean the relativistic quantum mechanics is saved. Firstly, Dirac equation doesn't replace the Klein-Gordon equation since they each describe different particles. Klein-Gordon equation describes *zero-spin* particles (thus it can really describe the electron despite the fact it was historically developed for that purpose!) and Dirac equation describes $\frac{1}{2} - spin$ particles. Moreover, for both Klein-Gordon and Dirac equation we have to deal with negative energy solutions. In the case of Dirac equation there is the famous reasoning from which we conclude the existence of anti-electrons, i.e. positrons. The solution proposed by Dirac is that all the negative energy solutions are already filled and since fermions obey the Pauli principle[1] there is actually a lower bound energy for the solutions of the Dirac equation. The problem is that this reasoning can't be applied for the case of the Klein-Gordon equation since bosons ignore the Pauli principle.

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

Definition 3. *Suppose we understand what is meant by a cause C and an 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 $t_E > |x_E|$.*

───────────────

[1]Pauli principle says that two identical fermions can't occupy the same quantum state.

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

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

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

$$A_1 = \langle x_1| e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t'} |x_0\rangle = \int_{\mathbb{R}} dp \ \langle x_1| e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t'} |p\rangle \langle p|x_0\rangle =$$

$$= \int_{\mathbb{R}} \frac{dp}{2\pi\hbar} \ e^{-\frac{i}{\hbar}\frac{p^2}{2m}t'} \langle x_1|p\rangle \langle p|x_0\rangle = \int_{\mathbb{R}} dp \ e^{-\frac{i}{\hbar}\frac{p^2}{2m}t'} e^{\frac{i}{\hbar}p(x_1-x_0)} =$$

$$= \int_{\mathbb{R}} \frac{dp}{2\pi\hbar} \ e^{-\frac{i}{\hbar}\left[\frac{p^2}{2m}t'-p(x_1-x_0)\right]} = \left|\begin{array}{c} \left[\frac{p^2}{2m}t' - p(x_1 - x_0)\right] = \\ \frac{t'}{2m}\left[p - \frac{m}{t'}(x_1 - x_0)\right]^2 - \frac{m}{2t'}(x_1 - x_0)^2 \end{array}\right| =$$

$$= e^{\frac{im}{2\hbar t'}(x_1-x_0)^2} \int_{\mathbb{R}} \frac{dp}{2\pi\hbar} \ e^{-\frac{it'}{2\hbar m}\left[p - \frac{m}{t'}(x_1-x_0)\right]^2}$$

In the integral we can substitute $p \to p + -\frac{m}{t'}(x_1 - x_0)$ so that the boudaries remain unchanged. Now the problem is that with the pure imaginary exponent we have an oscillatory function with no other term to guarantee the integral converges. As was shown in [8], we can actually use the trick of *rotating* the p in the complex plane by $\frac{\pi}{4}$ and get a known form of a gaussian integral multiplied by the phase factor.

$$= \left|p = e^{\frac{-i\pi}{4}}r \, dp = e^{\frac{-i\pi}{4}}dr\right| = e^{\frac{i\pi}{4}} e^{\frac{im}{2\hbar t'}(x_1-x_0)^2} \int_{\mathbb{R}} \frac{dp}{2\pi\hbar} \ e^{-\frac{t'}{2\hbar m}r^2}$$

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

From the final result 2.11 we see that the probability density of meassuring the transition $(x_0, 0) \to (x_1, t')$ 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

$$A_2 = \langle x_1| \, e^{-\frac{i}{\hbar}c\sqrt{\hat{p}^2+(mc)^2}t'} \, |x_0\rangle = \int_{\mathbb{R}} dp \, \langle x_1| \, e^{-\frac{i}{\hbar}c\sqrt{p^2+(mc)^2}t'} \, |p\rangle \, \langle p|x_0\rangle =$$

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

Let's analyze this integral in two ways. Firstly, let's try to solve the problem numerically to get the idea of how the integral behaves. The problem is similiar we had to deal with within the previous integral. The integrated function is oscillatory and thus the convergence is not expected in general. Numerically, we'll try to deal with that problem by choosing suitable boudaries. The best choice seems to be $p \in (-mc, mc)$ since it setups the desired condition on the *velocity* to be smaller then the speed of light. Then we only need to split the integral into a real and imaginary part.

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

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

$$\rightarrow \int_{-mc}^{mc} \frac{dp}{2\pi\hbar} \left[\sin(k)\sin(l) - \sin(k)\sin(l) + i\big(\sin(k)\cos(l) + \cos(k)\sin(l)\big) \right]$$

Now, we can integrate the function numerically using the Python[2] program 1 because we integrate the real part and the imaginary part separately. The graph contains the final probability amplitude.

_____

[2]The script uses *scipy*, *matplotlib* and *numpy* packages. The used interpretter was *cpython*, version 2.7
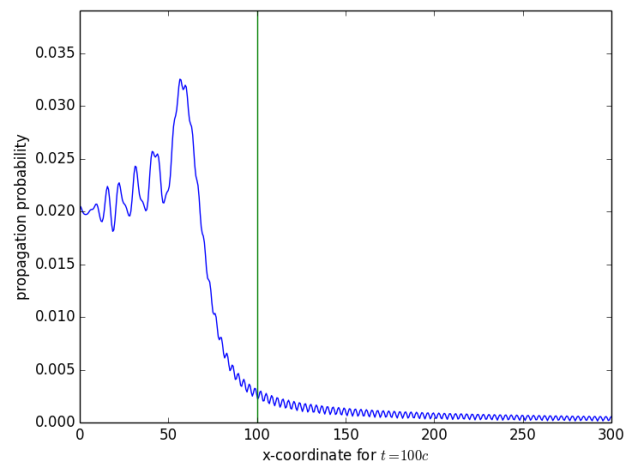
Figure 2.1: Propagation amplitude for a free relativistic particle

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

```python
from numpy import sqrt, cos, sin, linspace, exp, pi
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 1 / (2 * pi * hbar) * (
            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 1 / (2 * pi * hbar) * (
            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 * m, c * m)
    i = integrate.quad(imaginary, -c * m, c * m)
    y_list.append(sqrt(r[0] ** 2 + i[0] ** 2) / 2)

plt.xlabel("x-coordinate for $t = {}c$".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()
```

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 problem of the numericall approach is we have to deal with the non-zero error of the computation. To make sure the integral is non-zero in the region outside of the lightcone we will investigate the integrall analytically using the *steepest descent method*. Let $S(p)$ be the exponent part of the integrated function and $\Delta x = x_1 - x_0$. During the computation we will assume $(\Delta x)^2 > (ct')^2$ to take into account that we investigate the region where the amplitude should be zero.

$$S(p) = -\frac{i}{\hbar}c\sqrt{p^2 + (mc)^2}t' + \frac{i}{\hbar}p\Delta x$$

Now we should find the saddle points of S.

$$\frac{\partial S(p)}{\partial p} = 0$$

$$p^2 = \frac{(mc\Delta x)^2}{(ct')^2 - (\Delta x)^2}, \ p_\pm = \pm\frac{imc\Delta x}{\sqrt{(\Delta x)^2 - (ct')^2}}$$

Now we will investigate whether the values p_+, p_- are saddle points by finding the Hessian $\frac{\partial^2 S(p)}{\partial p^2}$.

$$\frac{\partial^2 S(p)}{\partial p^2} = \pm i\frac{\left((\Delta x)^2 - (ct')^2\right)^{\frac{3}{2}}}{m(ct')^2}$$

TODO: why to pick the $+$ solution? Thus we can conclude the amplitude A_2 is

$$A_2 \sim e^{S(p_+)} = e^{-\frac{mc}{\hbar}\sqrt{(\Delta x)^2 - (ct')^2}} \tag{2.13}$$

The expression 2.13 is non-zero for an arbitrary choice of Δx and t' thus it is non-zero also in the region outside of the lightcone. Thus we see we deal with the same problem again. The difference is that now we deal with an unexplainable 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

In the first chapter we tried to make a smooth transition from the "classical" quantum mechanics to the relativistic one by considering the rules of the *first quantization*. Our motivation was to use preserve the notations from the old theory, i.e. remain with the wavefunction being the mathematical object representing the physical state and operators corresponding to the dynamical variables. As was shown in the second chapter using this approach we must deal a number of various conceptual problems like negative probabilities or the break of causality.

Let's start with an observation. Using the canonical quantization we replaced each momentum, position and energy variable with the corresponding operator. So there is an operator for the position but not a single word was mentioned about the time. Why do we have a position operator but not a time operator? The time in all the equations was just a parameter. This assymetry between the time and space seems to be an another nail in the coffin of the first quantization. When searching for the the correct relativistic quantum thery we should seek such objects that treat space-time variables on the same footing.

3.1   Scalar fields

Let's start with the classical *Lagrangian* function L. Langragian L is being defined as a function $L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t)$ describing the evolution of $(q_1(t), \ldots, q_n(t), \dot{q}_1(t), \ldots, \dot{q}_n(t))$ in the configuration space using the least action principle $\delta S = 0$,

$$S = \int dt \, L(q_1(t), \ldots, q_n(t), \dot{q}_1(t), \ldots, \dot{q}_n(t)) \tag{3.1}$$

Now we want to investigate the dynamics of a field $\phi(\vec{x}, t)$ using the *Lagrangian density* $\mathcal{L}(\phi, \frac{\partial \phi}{\partial \vec{x}}, \frac{\partial \phi}{\partial t}, \ldots)$ instead.

$$L = \int d\vec{x} \, \mathcal{L}(\phi, \frac{\partial \phi}{\partial \vec{x}}, \frac{\partial \phi}{\partial t}, \frac{\partial^2 \phi}{\partial \vec{x}^2}, \frac{\partial^2 \phi}{\partial t^2} \dots) \tag{3.2}$$

From now, we will deal with time t and space $\vec{x}$ using the convenient relativistic notation

$$x^\mu = (ct, x^1, x^2, x^3)$$

and the 4-gradient is given by

$$\partial_\mu = (\frac{1}{c}\frac{\partial}{\partial t}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3})$$

As was shown in [10] using the Lagrangian $\mathcal{L} = \mathcal{L}(\phi, \partial_\mu \phi)$ the dynamics of ϕ is given by the equation

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right] = 0 \tag{3.3}$$

TODO: show the lorentz invariance of the euler legrange eq

Now we will investigate a simple example of the lagrangian which will come in use later. TODO: units discussions

$$\mathcal{L} = \frac{1}{2}\partial_\mu \phi \partial^\mu \phi + \frac{1}{2}m^2\phi^2 \tag{3.4}$$

Let's find the the equation for the Lagrangian 3.4 using 3.3.
TODO: klein-gordon field

$$\frac{\partial \mathcal{L}}{\partial \phi} = m^2\phi \partial_\mu \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right] = \partial^\mu \partial_\mu \phi$$

TODO: klein-gordon solution

3.2 Second quantization

TODO: a and a dagger operators

In this place I would like to cite a nice recipe from [9] which summarizes the canonical quantization we will use for going from a classical field theory to the quantum field theory:

- **Step I**: Write down a classical Lagrangian density in terms of fields. This is the creative part because there are lots of possible Lagrangians. After this step, everything else is automatic.

- **Step II**: Calculate the momentum density and work out the Hamiltonian density in terms of fields.

- **Step III**: Now treat the fields and momentum density as operators. Impose commutation relations on them to make them quantum mechanical.

- **Step IV**: Expand the fields in terms of creation/annihilation operators. This will allow us to use occupation numbers and stay sane.

- **Step V**: That's it. Congratulations, you are now the proud owner of a working quantum field theory, provided you remember the normal ordering interpretation.

TODO: quantize klein-gordon field

3.3   Causality problem

TODO: causality using the klein-gordon field

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

[8] Scipp.ucsc.edu. (2018). *A Gaussian integral with a purely imaginary argument*. [online] Available at: http://scipp.ucsc.edu/ haber/ph215/Gaussian.pdf [Accessed 13 May 2019].

[9] Lancaster, T. and Blundell, S. (2018). *Quantum field theory for the gifted amateur*. Oxford: Oxford University Press.

[10] Lancaster, T. and Blundell, S. (2018). *Quantum field theory for the gifted amateur*. Oxford: Oxford University Press.