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Bakalářská práce

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Aspekty přechodu od kvantové mechaniky ke kvantové teorii pole

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Milan Suk

Vedoucí práce: doc. Klaus Bering Larsen, Ph.D **Brno 2019**

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Autor:	Milan Suk Přírodovědecká fakulta, Masarykova univerzita Ústav teoretické fyziky a astrofyziky
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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 2019 ....

Milan Suk

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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 spin-less 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* $(\vec{q_1}, \ldots, \vec{q_n}, \vec{p_1}, \ldots, \vec{p_n})$. 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 phase 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*

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

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.

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

□

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

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

That means that if we have dynamical variables A and B we can get their quantum counterparts $\hat{A}$ 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 position space and H the corresponding Hilbert space. The quantization map is*

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

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*
$$Q(\{A, B\}) = \frac{1}{i\hbar}[\hat{A}, \hat{B}] \tag{1.6}$$
4. *a complete set $\{f_1, \dots, f_n\}$ is mapped to a complete set $\{Q(f_1), \dots, Q(f_n)\}$,*
5. *an identity $Id_{\mathcal{Q}}$ is mapped to the identity $Id_H = Q(Id_{\mathcal{Q}})$*

It is convenient 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: $[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B, C] + [A, C]B$

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

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

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

Groenewold theorem Although 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

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

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

now we should find the corresponding operators.

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

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

$$\Big[Q(\hat{x}^2\hat{p}), Q(\hat{x}\hat{p})\Big] = \frac{1}{4}\Big(\big[\hat{x}^2\hat{p}, \hat{x}\hat{p}\big] + \big[\hat{x}^2\hat{p}, \hat{p}\hat{x}\big] + \big[\hat{p}\hat{x}^2, \hat{x}\hat{p}\big] + \big[\hat{p}\hat{x}^2, \hat{p}\hat{x}\big]\Big) =$$
$$\frac{i\hbar}{2}\Big(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2 + [\hat{x}, \hat{p}]\hat{x}\Big) = \frac{i\hbar}{2}\Big(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2\Big) - \hbar^2\hat{x}$$

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 approximation.

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

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

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 heuristic approach for the 1st quantization and simply use the following quantization rules for momentum 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 spin-less 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 $Q(\vec{p}^2) = -\hbar^2\Delta$.

$$\begin{aligned} E^2 &= \vec{p}^2c^2 + m^2c^4 \\ -\hbar^2\frac{\partial^2}{\partial t^2}\psi &= -\hbar^2c^2\Delta\psi + m^2c^4\psi \end{aligned}$$

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

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

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 $(\hat{K}' + \mathbb{I}\mu)(\hat{K}' - \mathbb{I}\mu) = \big(\hat{K}'\big)^2 - \mu^2$.

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

and by rewriting the expression above we get

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

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 $i \neq j \wedge i, j \in \{1, 2, 3\}$. To satisfy all these conditions γ^μ is clearly not a number. When Dirac was deriving the equation he immediately recognized the gammas to be 4x4 matrices. One example of such a set of matrices is the Dirac representation.

$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$
$$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Let's check these matrices work correctly with all the equations $(\gamma^0)^2 = 1$, $(\gamma^i)^2 = -1$ and $\gamma^i\gamma^j + \gamma^j\gamma^i = 0$. We can also notice that last three matrices are composed from sub-matrices of the from of Pauli's matrices.

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For Pauli matrices there is the same relation we found for the gamma matrices $\sigma^i\sigma^j + \sigma^j\sigma^i = 2\delta_{ij}\mathbb{I}_{2\times2}$. Without knowing the exact form of Pauli matrices and taking only the anti-commutation relation we can prove the defining property holds if we rewrite the gamma matrices using a compact form with sub-matrices.

$$\gamma^i = \begin{pmatrix} 0_{2\times2} & \sigma^i \\ -\sigma^i & 0_{2\times2} \end{pmatrix} \quad \Longrightarrow$$
$$\gamma^i\gamma^j = \begin{pmatrix} 0_{2\times2} & \sigma^i \\ -\sigma^i & 0_{2\times2} \end{pmatrix} \begin{pmatrix} 0_{2\times2} & \sigma^j \\ -\sigma^j & 0_{2\times2} \end{pmatrix} = -\begin{pmatrix} \sigma^i\sigma^j & 0_{2\times2} \\ 0_{2\times2} & \sigma^i\sigma^j \end{pmatrix} =$$

Thus we can write $\gamma^i\gamma^j + \gamma^j\gamma^i = \{\gamma^i, \gamma^j\}$ using $\{\sigma^i, \sigma^j\}$ terms.

$$\{\gamma^i, \gamma^j\} = -\begin{pmatrix} \sigma^i\sigma^j & 0_{2\times2} \\ 0_{2\times2} & \sigma^i\sigma^j \end{pmatrix} - \begin{pmatrix} \sigma^j\sigma^i & 0_{2\times2} \\ 0_{2\times2} & \sigma^j\sigma^i \end{pmatrix} = -\begin{pmatrix} \{\sigma^i, \sigma^j\} & 0_{2\times2} \\ 0_{2\times2} & \{\sigma^i, \sigma^j\} \end{pmatrix} = -2\delta_{ij}\mathbb{I}_{4\times4}$$

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

2.1.1 Schrödinger's equation

In the non-relativistic case we can find the continuity equation by taking the complex conjugate of the Schrödinger'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 multiply 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 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 $\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$.

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

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

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

2.1.2 Klein-Gordon equation

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 subtract 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 proportional 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 interpretation of ρ as the *probability density of measuring the system within a given state* ψ. To solve this problem, Dirac introduced his equation.

2.1.3 Dirac 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])*

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

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.

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

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.

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

□

We will use a similar trick we used within the Schrödinger's 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

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

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

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! Unfortunately 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. Let's start by discussing

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

the definition of the causality. Causality is relationship between a cause and an effect. Naively, it feels reasonable to expect two events to not be causal if they happen in a great distance from each other or within a big time difference. Since a massive object always travel with a lower speed then a speed of light it makes sense to setup the condition of causality using the speed of light. Basically, if it is possible for an object with a configuration $X_1 = (x_1, ct_1)$ to get to the point $X_2 = (x_2, ct_2)$ then there might be a causality between X_1 and X_2.

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 light cone 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

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

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

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

In the integral we can substitute $p \to p + -\frac{m}{t'}(x_1 - x_0)$ so that the boundaries 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 measuring 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 light cone 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 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 similar 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 boundaries. 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.

$$\int_{\mathbb{R}} \frac{dp}{2\pi\hbar} \; e^{-\frac{i}{\hbar}c\sqrt{p^2+(mc)^2}t'} e^{\frac{i}{\hbar}p(x_1 - x_0)} =$$
$$= \left| \begin{matrix} k_{t'}(p) = -\frac{1}{\hbar}c\sqrt{p^2 + (mc)^2}t' \\ l_{x_1}(p) = \frac{1}{\hbar}p(x_1 - x_0) \end{matrix} \right| \to$$
$$\to \int_{-mc}^{mc} \frac{dp}{2\pi\hbar} \left[\sin(k)\sin(l) - \sin(k)\sin(l) + i\big(\sin(k)\cos(l) + \cos(k)\sin(l)\big) \right]$$

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.

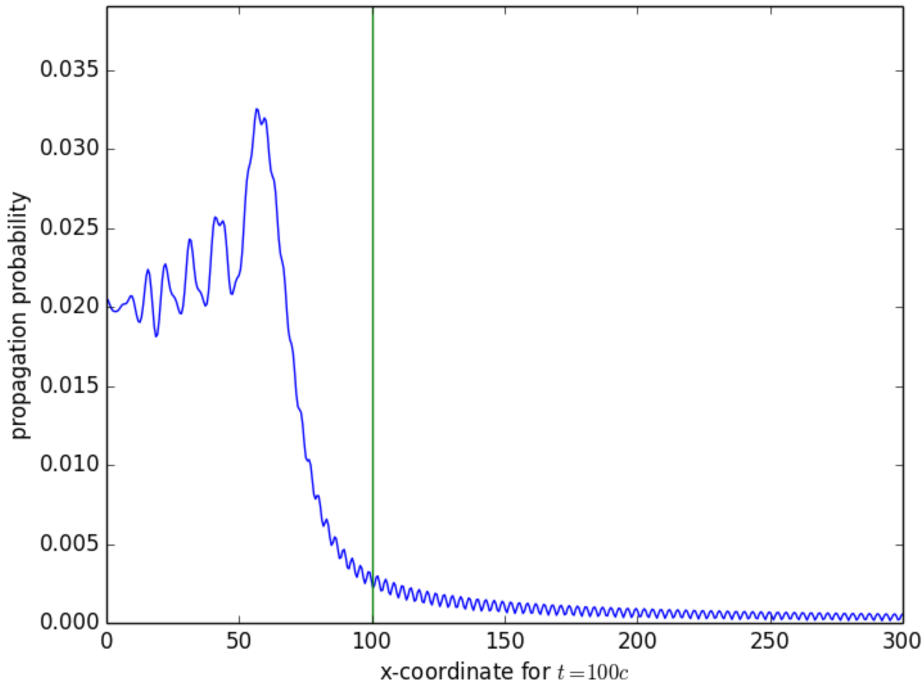

Figure 2.1: Propagation amplitude for a free relativistic particle

[2]The script uses *scipy*, *matplotlib* and *numpy* packages. The used interpreter was *cpython*, version 2.7

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

```
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. Although the value in the graph is reaching the zero very quickly it is very small but non-zero in the region outside of the light cone (i.e. on the right side of the vertical marking line). So we encounter the same problem as in the calculation with the non-relativistic particle. The problem of the numerical 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 light cone we will investigate the integral 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. Also for the calculation we will wick rotate the time using $t' = t_M = -it_E$.

$$S(p) = -\hbar c\sqrt{p^2 + (mc)^2} t_E + \frac{i}{\hbar} p\Delta x$$

Now we should find the saddle points of S.

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

$$p^2 = \frac{(mc\Delta x)^2}{(ct_E)^2 + (\Delta x)^2}, \; p_\pm = \pm \frac{imc\Delta x}{\sqrt{(\Delta x)^2 + (ct_E)^2}}$$

We have to make sure whether the values p_+, p_- are saddle points. Let's plug the solution back into $\frac{\partial S(p)}{\partial p}$.

$$\left.\frac{\partial S(p)}{\partial p}\right|_{p=p_\pm} = -c\frac{\pm i\Delta x mct_E}{\sqrt{(ct_E)^2 + (\Delta x)^2}} \cdot \sqrt{\frac{(ct_E)^2 + (\Delta x)^2}{(mc^2 t_E)^2}} + i\Delta x = \mp i\Delta x + i\Delta x$$

From this result we can conclude the only point satifying the equation $\frac{\partial S(p)}{\partial p} = 0$ is p_+. Now we find the value of the Hessian $\frac{\partial^2 S(p)}{\partial p^2}$ in the saddle point p_+.

$$H = \left.\frac{\partial^2 S(p)}{\partial p^2}\right|_{p=p_+} = \frac{\left((ct_E)^2 + (\Delta x)^2\right)^{\frac{3}{2}}}{c^3 m t^2}$$

After ratating the time back $t_E \to t_M = t'$ we can conclude the amplitude A_2 is

$$A_2 \approx e^{S(p_+)}\sqrt{\frac{2\pi}{-H}} = e^{-\frac{mc}{\hbar}\sqrt{(\Delta x)^2 - (ct')^2}} \sqrt{\frac{2\pi c^3 m t^2}{\left((\Delta x)^2 - (ct')^2\right)^{\frac{3}{2}}}} \tag{2.13}$$

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 light cone. 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 wave function 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 asymmetry between the time and space seems to be an another nail in the coffin of the first quantization. When searching for the correct relativistic quantum theory 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. Lagrangian 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.

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

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

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

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. Also, since it is a standard in the literature to use the *natural units* we will also set $\hbar = 1$ and $c = 1$ and if needed the constants can be retrieved using the dimensional analysis.

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

Let's find the equation for the Lagrangian 3.4 using 3.3.

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

The equation for the field ϕ takes the form 3.5 and is very similar to the Klein-Gordon equation from the first chapter!

$$\partial^\mu \partial_\mu \phi + m^2 \phi = 0 \tag{3.5}$$

We will find a solution of this equation using the Fourier transformation of ϕ.

$$\phi(\vec{x}, t) = \int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3}\, e^{i\vec{p}\vec{x}}\, \phi(\vec{p}, t) \tag{3.6}$$

The equation 3.5 then becomes

$$(\partial^\mu \partial_\mu + m^2) \int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3}\, e^{i\vec{p}\vec{x}}\, \phi(\vec{p}, t) = 0$$
$$\int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3}\, (\partial_t^2 - \Delta + m^2)\, e^{i\vec{p}\vec{x}}\, \phi(\vec{p}, t) = 0$$
$$\int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3}\, (\partial_t^2 + |\vec{p}|^2 + m^2)\, e^{i\vec{p}\vec{x}}\, \phi(\vec{p}, t) = 0$$

which results in the equation

$$(\partial_t^2 + |\vec{p}|^2 + m^2)\phi(\vec{p}, t) = 0$$

Thus we see the dispersion relation is $\omega^2 = |\vec{p}|^2 + m^2$. We should seek the solution in form of combination of $a_p e^{i\vec{p}\vec{x}}$.

$$\phi(\vec{x}, t) = \int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3\sqrt{2\omega_p}} \left[ae^{i\vec{p}\vec{x}} + a'e^{-i\vec{p}\vec{x}}\right]$$

In the correspondence with the classical Lagrangian, Hamiltonian and momentum, we can also define Hamiltonian density and "momentum density". Let's denote $\dot{\phi} = \partial_t \phi$.

$$\Pi(\vec{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}}$$
$$\mathcal{H} = \Pi(\vec{x}, t) \cdot \dot{\phi}(\vec{x}, t) - \mathcal{L}$$

In the case of the free scalar field 3.4 the Π is given by

$$\Pi(\vec{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \frac{\partial}{\partial \dot{\phi}}\left[\frac{1}{2}\partial_\mu \phi \partial^\mu \phi - \frac{1}{2}m^2\phi^2\right] = \dot{\phi}$$

which we can use the see the form of the Hamiltonian density.

$$\mathcal{H} = \dot{\phi}^2 - \frac{1}{2}\left[\partial_\mu \phi \partial^\mu \phi - m^2\phi^2\right] = \dot{\phi}^2 - \frac{1}{2}\left[\dot{\phi}^2 - \left(\nabla\phi\right)^2 - m^2\phi^2\right] =$$
$$\frac{1}{2}\left[\dot{\phi}^2 + \left(\nabla\phi\right)^2 + m^2\phi^2\right]$$

3.2 Second quantization

In the procedure of second quantization we must start with the representation of the state of the system. We will use the *occupation number representation* which counts the number of particles in each state. We will write the *vacuum state* as $|0\rangle = |\ldots, 0, \ldots\rangle$. The general state $|n_1, \ldots, n_N\rangle$ represents the system with n_1 particles in the first state, etc. In the analogy with the harmonic oscillator we will introduce *creation* and *annihilation* operators $\hat{a}_{\vec{p}}$ and $\hat{a}_{\vec{p}}^\dagger$. The basic properties are that $\hat{a}_{\vec{p}}$ annihilates the vacuum state and $\hat{a}_{\vec{p}}^\dagger$ creates the $|\vec{p}\rangle$ state.

$$\hat{a}_{\vec{p}}\,|0\rangle = 0$$
$$\hat{a}_{\vec{p}}^\dagger\,|0\rangle = |\vec{p}\rangle$$

The commutation relations are

$$\left[\hat{a}_{\vec{p}}, \hat{a}_{\vec{p}'}\right] = \left[\hat{a}_{\vec{p}}^\dagger, \hat{a}_{\vec{p}'}^\dagger\right] = 0$$
$$\left[\hat{a}_{\vec{p}}, \hat{a}_{\vec{p}'}^\dagger\right] = (2\pi)^3\delta(\vec{p} - \vec{p}')$$

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.

Let's rewrite the Klein-Gordon field with the creation and annihilation operator to promote the ϕ field to the field operator. We expect the ϕ and Π field to have commutation relation in the same form as they had in the discrete case. But instead of discrete δ^μ_ν matrix we should use the Dirac delta function.

$$\begin{gathered}\big[\phi(x), \phi(x')\big] = \big[\Pi(x), \Pi(x')\big] = 0 \\ \big[\phi(x), \Pi(x')\big] = i\delta(x - x')\end{gathered}$$

The first one will be shown in the next section for the case of a time-like space-time events. The second one can be calculated directly using the scalar field obtained in the previous part. But we will replace the constants $a_p \to \hat{a}_p$, $a'_p \to \hat{a}^\dagger_p$ and check whether the choice is fine by the commutator value.

$$\begin{gathered}\big[\phi(x), \Pi(x')\big] = \\ \left[\int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3\sqrt{2\omega_p}} \left(\hat{a}_p e^{ipx} + \hat{a}^\dagger_p e^{-ipx}\right), \int_{\mathbb{R}^3} \frac{dp'^3}{(2\pi)^3}(-i)\sqrt{\frac{\omega_{p'}}{2}} \left(\hat{a}_{p'} e^{ip'x'} - \hat{a}^\dagger_{p'} e^{-ip'x'}\right)\right] =\end{gathered}$$

There is a little trick that we replace $\hat{a}^\dagger_p e^{-ipx}$ by $\hat{a}^\dagger_{-p} e^{ipx}$. After this we will use the commutation relation for $\hat{a}_p$ and $\hat{a}^\dagger_p$ to simplify the commutator significantly.

$$\begin{gathered}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3 dp'^3}{(2\pi)^6} \frac{(-i)}{2} \sqrt{\frac{\omega_{p'}}{\omega_p}} \left[\hat{a}_p e^{ipx} + \hat{a}^\dagger_{-p} e^{ipx}, \hat{a}_{p'} e^{ip'x'} - \hat{a}^\dagger_{-p'} e^{ip'x'}\right] = \\ \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3 dp'^3}{(2\pi)^6} \frac{(-i)}{2} \sqrt{\frac{\omega_{p'}}{\omega_p}} \Big(- \big[\hat{a}_{p'}, \hat{a}^\dagger_{-p}\big] - \big[\hat{a}_p, \hat{a}^\dagger_{-p'}\big]\Big) e^{ip'x' + ipx} =\end{gathered}$$

Finally, let's replace the commutators with the delta functions $\big[\hat{a}_p, \hat{a}^\dagger_{p'}\big] = (2\pi)^3\delta(p - p')$.

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3 dp'^3}{(2\pi)^3}\frac{i}{2}\sqrt{\frac{\omega_{p'}}{\omega_p}}\Big(\delta(p'+p)+\delta(p'+p)\Big)e^{ip'x'+ipx} =$$
$$\int_{\mathbb{R}^3}\frac{dp^3}{(2\pi)^3} i e^{-ip(x'-x)} = i\delta(x-x')$$

3.3 Causality problem

Now we shall check whether the new formulation for a free scalar relativistic theory gives the right results about causality. The first thing we could do is basically calculate the propagator $\langle 0|\,\hat{\phi}(x)\hat{\phi}(y)\,|0\rangle$ and hope the value will be zero outside of the light cone. But, instead we should go back and check whether our condition for the causality is still valid in the case of the quantum field theory. We know that if two observables A and B are being measured we can decide whether the measurement of A influences the value of B by calculating their commutator $[A,B]$. It is important that if $[A,B]\neq 0$ then by measuring A it is possible to decide whether B has bee measured on the system or not and vice versa.

This means that when $[A,B]\neq 0$ the event must be time-like[1] since they are *correlated*. If $[A,B]=0$ then there is no information of possible measurement B when doing the measurement A and thus the event might be space-like and it doesn't matter we could do a transformation into a frame such that we reverse the order of the events.

Definition 4. *Causality is not preserved if for a space-like separated points x, y the field operator doesn't commute with itself in these points, i.e. we can simultaneously measure values which are correlated and the time ordering is not preserved for different frames. Technically for $(x-y)\eta(x-y)<0$*

$$\big[\phi(x),\phi(y)\big]\neq 0 \tag{3.7}$$

So to check the causality we will check the commutator $[\phi(x),\phi(y)]$.

[1] *Time-like* separated events are inside of the light cone of each other. *Space-like* separated events are outside of the light cone of each other and thus the Lorentz transformation of those events does not preserve time ordering.

$$\Big[\phi(x), \phi(x')\Big] =$$
$$\Big[\int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \big(\hat{a}_p e^{ipx} + \hat{a}_p^\dagger e^{-ipx}\big), \int_{\mathbb{R}^3} \frac{dp'^3}{(2\pi)^3} \frac{1}{\sqrt{2\omega_{p'}}} \big(\hat{a}_{p'} e^{ip'x'} + \hat{a}_{p'}^\dagger e^{-ip'x'}\big)\Big] =$$
$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3\, dp'^2}{(2\pi)^6} \frac{1}{2\sqrt{\omega_p \omega_{p'}}} \Big[\hat{a}_p e^{ipx} + \hat{a}_p^\dagger e^{-ipx}, \hat{a}_{p'} e^{ip'x'} + \hat{a}_{p'}^\dagger e^{-ip'x'}\Big] =$$
$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3\, dp'^2}{(2\pi)^6} \frac{1}{2\sqrt{\omega_p \omega_{p'}}} \Big(\big[\hat{a}_p e^{ipx}, \hat{a}_{p'}^\dagger e^{-ip'x'}\big] + \big[\hat{a}_p^\dagger e^{-ipx}, \hat{a}_{p'} e^{ip'x'}\big]\Big) =$$
$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{dp^3\, dp'^2}{(2\pi)^3} \frac{1}{2\sqrt{\omega_p \omega_{p'}}} \big(\delta(p-p') e^{ipx - ip'x'} - \delta(p-p') e^{-(ipx - ip'x')}\big) =$$
$$\int_{\mathbb{R}^3} \frac{dp^3}{(2\pi)^3} \frac{1}{2\omega_{p'}} \big(e^{ip(x-x')} - e^{-ip(x-x')}\big)$$

Now, as discussed in [3], there is the trick doing the Lorentz transformation of the second term $-(x-y) \to (x-y)$[2] for case $x-y$ in the case the $x-y$ is space-like. Since it is a Lorentz invariant, terms in the integral cancel each other and thus the commutator is zero. Inside of the light cone, we don't have such a continuous transformation because we would have to map a point from the future light cone to the past light cone. Because of that the commutator is non-zero for the time-like separated points which means inside of the light cone events might be causal.

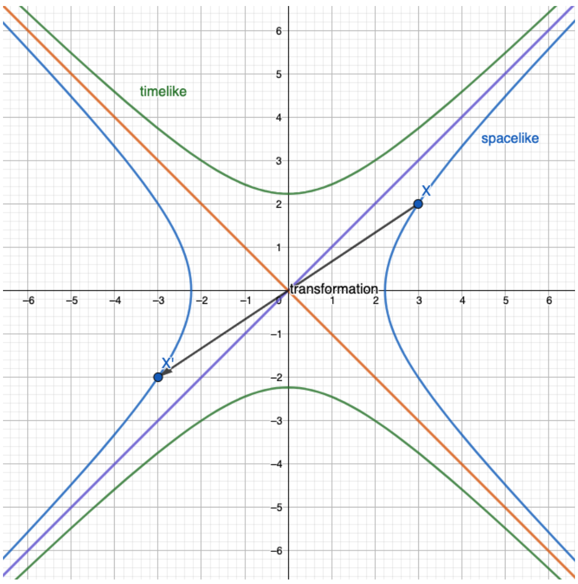

Figure 3.1: Lorentz transformation of the space-like event.

[2]Clearly $-\mathbb{I}$ is the desired inversion $x^\mu \to -x^\mu = (-\delta^\mu_\nu)x^\nu$ and it is a Lorentz transformation because $(-\mathbb{I})\eta(-\mathbb{I}^T) = \eta$. Also we can see geometrically Lorentz transformation is moving the point on the sphere of the hyperboloid outside of the light cone but there is no continuous map between the hyperbolas in the future light cone and the past cone.

Conclusion

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