Klein-Gordon equation

8.1 Introduction

The construction of quantum mechanics, which considers time as decoupled from space variables, is not compatible with the principles of special relativity. Additionally, experimental observations show that quantum mechanics is only accurate when the observed phenomena involve particles at low speeds. For example, it is not a suitable model for describing experiments involving interaction between light and matter.
In this chapter, we introduce the initial efforts to modify quantum mechanics to incorporate relativistic principles. Our first objective will be to derive a relativistic equation. In other words, we will begin our exploration with a particle that possesses zero spin. Within this context, it is logical to operate within the framework of Minkowski space, which is fundamental to special relativity, in order to develop a relativistic theory.
In order to describe quantum particles with zero spin and relativistic speeds, the Klein-Gordon equation is introduced. This equation is the relativistic equivalent of the Schrödinger equation given by,

$$H\psi = E\psi \tag{8.1}$$

By applying the principle of equivalence, we can write

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{\overrightarrow{P}^2}{2m}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi, \qquad \overrightarrow{p} = -i\hbar\overrightarrow{\nabla} \tag{8.2}$$

It is known that in the case of plane waves, the functions $\psi(\overrightarrow{r}, t)$ which are solutions of the Schrödinger equation are given by.

$$\psi(\overrightarrow{r}, t) = e^{i(\frac{\overrightarrow{p}\cdot\overrightarrow{r}}{\hbar} - \frac{E\cdot t}{\hbar})} \tag{8.3}$$

Let's attempt to find the general form of the Klein-Gordon equation, which allows us to describe the motion of free particles with zero spin and relativistic velocities, starting from the Schrödinger equation.

8.2 Quadri-vectors in field theory.

It is important to remember that the relativistic energy of a free particle is determined by

$$E = \sqrt{\overrightarrow{p}^2 c^2 + m^2 c^4} \tag{8.4}$$

- $\overrightarrow{p}$: impulsion
- c : velocity of light
- m : mass of the particle

The energy-momentum quadri-vector $\overrightarrow{P}$ is defined by.

$$\overrightarrow{\mathbf{P}} = \left(\overrightarrow{p}, \frac{E}{c}\right) \tag{8.5}$$

In field theory, the Einstein convention is used. If $\overrightarrow{A}$ is a quadri-vector, it is denoted as A_μ with $\mu = 1, 2, 3, 4$. The quadri-vector A_μ has the following components:

$$A_\mu = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ ia_4 \end{pmatrix} \tag{8.6}$$

When calculating the dot product of two quadri-vectors A_μ and B_ν, the result is obtained

$$A_\mu B_\nu = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ ia_4 \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ ib_4 \end{pmatrix} = +a_1 b_1 + a_2 b_2 + a_3 b_3 - a_4 b_4 \tag{8.7}$$

The scalar product satisfies the metric of Minkowski space $(+, +, +, -)$.
In the field theory, the energy-momentum quadri-vector is written as:

$$P_\mu = \left(\overrightarrow{p}, i\frac{E}{c}\right) \tag{8.8}$$

It should be emphasized that in quantum mechanics, E and $\overrightarrow{p}$ are defined as:

$$E \to i\hbar\frac{\partial}{\partial t} \qquad \overrightarrow{p} \to -i\hbar\overrightarrow{\nabla} \tag{8.9}$$

By substituting (8.9) into (8.8), we obtain

$$P_\mu = \left(-i\hbar\overrightarrow{\nabla}, i\frac{i\hbar}{c}\frac{\partial}{\partial t}\right) = -i\hbar\left(\overrightarrow{\nabla}, -\frac{i}{c}\frac{\partial}{\partial t}\right) \tag{8.10}$$

If we set,

$$\partial_\mu = \left(\overrightarrow{\nabla}, -\frac{i}{c}\frac{\partial}{\partial t}\right) \tag{8.11}$$

The quadri-vector spatio-temporal derivative is represented by ∂_μ, where we find

$$P_\mu = -i\hbar\partial_\mu \tag{8.12}$$

8.3 Free Klein-Gordon equation

Let's now find the equation of the free Klein-Gordon describing the motion (displacement) of a quantum particle, with zero spin and relativistic speed
In quantum mechanics, a free particle is described by the Schrödinger's evolution equation.

$$i\hbar\frac{\partial}{\partial t}\phi(\overrightarrow{r},t) = E\phi(\overrightarrow{r},t) \quad \text{où} \quad E = H = E_c + V = E_c + 0 = \frac{1}{2}mv^2 \quad \text{avec} \quad v << c \tag{8.13}$$

For a free relativistic particle

$$E_R = \sqrt{\overrightarrow{p}^2c^2 + m^2c^4} \tag{8.14}$$

The dynamics of these relativistic particles will be described by the following equation

$$i\hbar\frac{\partial}{\partial t}\phi(\overrightarrow{r},t) = E_R \quad \phi(\overrightarrow{r},t) = \sqrt{\overrightarrow{p}^2c^2 + m^2c^4} \quad \phi(\overrightarrow{r},t) \tag{8.15}$$

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2 \phi(\overrightarrow{r},t) = \left(\sqrt{\overrightarrow{p}^2c^2 + m^2c^4}\right)^2 \quad \phi(\overrightarrow{r},t) \tag{8.16}$$

$$-\hbar^2\frac{\partial^2}{\partial^2 t}\phi(\overrightarrow{r},t) = \left(\overrightarrow{p}^2c^2 + m^2c^4\right) \quad \phi(\overrightarrow{r},t) \tag{8.17}$$

$$-\hbar^2 \frac{\partial^2}{\partial^2 t} \phi(\overrightarrow{r}, t) = \left(\left(-i\hbar \overrightarrow{\nabla} \right)^2 c^2 + m^2 c^4 \right) \quad \phi(\overrightarrow{r}, t) \tag{8.18}$$

$$-\hbar^2 \frac{\partial^2}{\partial^2 t} \phi(\overrightarrow{r}, t) = \left(\left(-i\hbar \overrightarrow{\nabla} \right)^2 c^2 + m^2 c^4 \right) \quad \phi(\overrightarrow{r}, t) \tag{8.19}$$

$$\frac{-\hbar^2}{\hbar^2 c^2} \frac{\partial^2}{\partial^2 t} \phi(\overrightarrow{r}, t) + \frac{\hbar^2 \overrightarrow{\nabla}^2 c^2}{\hbar^2 c^2} \quad \phi(\overrightarrow{r}, t) - \frac{m^2 c^4}{\hbar^2 c^2} \quad \phi(\overrightarrow{r}, t) = 0 \tag{8.20}$$

By setting $\overrightarrow{\nabla}^2 = \Delta$, we obtain the following equation

$$\left(\Delta - \frac{1}{c^2} \frac{\partial^2}{\partial^2 t} - \frac{m^2 c^2}{\hbar^2} \right) \quad \phi(\overrightarrow{r}, t) = 0 \tag{8.21}$$

The final equation represents the free Klein-Gordon equation written in real space. Let us now seek the form of this equation in Minkowski space.
We have

$$\partial_\mu = \left(\overrightarrow{\nabla}, -\frac{i}{c} \frac{\partial}{\partial t} \right) \Longrightarrow \partial_\mu^2 = \partial_\mu \cdot \partial_\mu = \left(\overrightarrow{\nabla}, -\frac{i}{c} \frac{\partial}{\partial t} \right) \cdot \left(\overrightarrow{\nabla}, -\frac{i}{c} \frac{\partial}{\partial t} \right) \tag{8.22}$$

$$\partial_\mu^2 = \left(\Delta, -\frac{1}{c^2} \frac{\partial^2}{\partial^2 t} \right) = \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial^2 t} \tag{8.23}$$

By replacing (8.23) in (8.21), we get

$$\left(\partial_\mu^2 - \frac{m^2 c^2}{\hbar^2} \right) \quad \phi(\overrightarrow{r}, t) = 0 \tag{8.24}$$

By setting $\hbar = c = 1$ and defining $(\overrightarrow{r}, t) = x_\mu$, where x_μ denotes a point in Minkowski space and $\mu = 1, 2, 3, 4$, the equation (8.24) is transformed

$$\left(\partial_\mu^2 - m^2 \right) \phi(x_\mu) = 0 \tag{8.25}$$

This equation represents the free Klein-Gordon equation expressed in Minkowski space.

8.4 Invariance of the free Klein-Gordon equation under gauge transformation

<u>**Exercice**</u> **6** :

The motion of a particle with mass m, zero spin, and relativistic speed c is governed by the following free Klein-Gordon equation

$$\left(\partial_\mu^2 - m^2\right)\phi(x_\mu) = 0$$

- Demonstrate the invariance of this equation under the following gauge transformation

$$\phi(x_\mu) \longrightarrow \phi'(x_\mu) = e^{-iq\alpha(x_\mu)}\phi(x_\mu) \quad , \quad \phi(x_\mu), \alpha(x_\mu) \quad \text{sont deux réels arbitraires.}$$

8.5 Solutions to the free Klein-Gordon equation

The free for Klein-Gordon equation is given by

$$\left(\partial_\mu^2 - m^2\right)\phi(x_\mu) = 0 \quad \text{qu'on peut écrire} \quad \left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial^2 t} - \frac{m^2c^2}{\hbar^2}\right) \quad \phi(\overrightarrow{r}, t) = 0 \tag{8.26}$$

This equation has a solution in steady states. Its general form is given by,

$$\phi(\overrightarrow{r}, t) = f(t) \cdot \psi(\overrightarrow{r}) \tag{8.27}$$

It is said that a steady-state solution is a solution with separable variables. Substituting (8.27) into (8.26), we find

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial^2 t} - \frac{m^2c^2}{\hbar^2}\right) \quad f(t) \cdot \psi(\overrightarrow{r}) = 0 \tag{8.28}$$

$$f(t)\Delta\psi(\overrightarrow{r}) - \psi(\overrightarrow{r})\frac{1}{c^2}\frac{\partial^2}{\partial^2 t}f(t) - \frac{m^2c^2}{\hbar^2}f(t)\psi(\overrightarrow{r}) = 0 \tag{8.29}$$

Dividing the entire equation by $f(t)\psi(\overrightarrow{r})$ yields

$$\frac{f(t)\Delta\psi(\overrightarrow{r})}{f(t)\psi(\overrightarrow{r})} - \frac{1}{f(t)\psi(\overrightarrow{r})}\psi(\overrightarrow{r})\frac{1}{c^2}\frac{\partial^2}{\partial^2 t}f(t) - \frac{1}{f(t)\psi(\overrightarrow{r})}\frac{m^2c^2}{\hbar^2}f(t)\psi(\overrightarrow{r}) = 0 \tag{8.30}$$

$$\frac{\Delta\psi(\overrightarrow{r})}{\psi(\overrightarrow{r})} - \frac{1}{f(t)}\frac{1}{c^2}\frac{\partial^2}{\partial^2 t}f(t) - \frac{m^2c^2}{\hbar^2} = 0 \tag{8.31}$$

This equation represents a second-order equation with two independent variables.

$$\frac{\Delta\psi(\overrightarrow{r})}{\psi(\overrightarrow{r})} - \frac{m^2c^2}{\hbar^2} = \frac{1}{c^2}\frac{f''(t)}{f(t)} = \text{constante}, \quad \text{avec} \quad f'' = \frac{\partial^2}{\partial^2 t}f(t) \tag{8.32}$$

If we define $constant = \omega^2$, we can deduce

$$\frac{\Delta\psi(\overrightarrow{r})}{\psi(\overrightarrow{r})} - \frac{m^2c^2}{\hbar^2} = \frac{1}{c^2}\frac{f''(t)}{f(t)} = \omega^2 \tag{8.33}$$

From this equation, we derive the two following equations:

$$\frac{\Delta\psi(\overrightarrow{r})}{\psi(\overrightarrow{r})} - \frac{m^2c^2}{\hbar^2} = \omega^2 \Longrightarrow \frac{\Delta\psi(\overrightarrow{r})}{\psi(\overrightarrow{r})} = \omega^2 + \frac{m^2c^2}{\hbar^2} \Longrightarrow \Delta\psi(\overrightarrow{r}) - \left(\omega^2 + \frac{m^2c^2}{\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \tag{8.34}$$

$$\frac{1}{c^2}\frac{f''(t)}{f(t)} = \omega^2 \Longrightarrow \frac{f''(t)}{f(t)} = c^2\omega^2 \Longrightarrow f''(t) = c^2\omega^2 f(t) \Longrightarrow f''(t) - c^2\omega^2 f(t) = 0 \tag{8.35}$$

Equation (8.35) can be expressed in the following general form

$$f''(t) \pm (c\omega)^2 f(t) = 0 \tag{8.36}$$

Equation (8.35) then has solutions of the form

$$f(t) = A\, e^{c\omega t} + B\, e^{-c\omega t} \tag{8.37}$$

In order to have continuous solutions everywhere, we set

$$c\,\omega = \frac{i\,E}{\hbar}, \quad E \text{ est un réel.} \tag{8.38}$$

By substituting (8.37) into (8.38), we obtain

$$f(t) = A\, e^{\frac{i\,E}{\hbar}\, t} + B\, e^{-\frac{i\,E}{\hbar}\, t} \tag{8.39}$$

We have

$$c\,\omega = \frac{i\,E}{\hbar} \Longrightarrow c^2\,\omega^2 = -\frac{E^2}{\hbar^2} \Longrightarrow \omega^2 = -\frac{E^2}{c^2\hbar^2} \tag{8.40}$$

Let us now substitute into equation (8.34)

$$\Delta\psi(\overrightarrow{r}) - \left(-\frac{E^2}{c^2\hbar^2} + \frac{m^2c^2}{\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \Longrightarrow \tag{8.41}$$

By finding a common denominator, one can determine

$$\Delta\psi(\overrightarrow{r}) - \left(-\frac{E^2}{c^2\hbar^2} + \frac{m^2c^4}{c^2\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \Longrightarrow \Delta\psi(\overrightarrow{r}) - \left(\frac{-E^2 + m^2c^4}{c^2\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \tag{8.42}$$

Or,

$$E^2 = \overrightarrow{p}^2c^2 + m^2c^4 \Longrightarrow -\overrightarrow{p}^2c^2 = -E^2 + m^2c^4 \tag{8.43}$$

By substituting into the previous equation, we find

$$\Delta\psi(\overrightarrow{r}) - \left(\frac{-\overrightarrow{p}^2c^2}{c^2\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \Longrightarrow \Delta\psi(\overrightarrow{r}) - \left(\frac{-\overrightarrow{p}^2}{\hbar^2}\right)\psi(\overrightarrow{r}) = 0 \Longrightarrow \tag{8.44}$$

$$\Delta\psi(\overrightarrow{r}) - \left(\frac{i\,\overrightarrow{p}}{\hbar}\right)^2\psi(\overrightarrow{r}) = 0 \tag{8.45}$$

This equation has solutions of the following form

$$\psi(\overrightarrow{r}) = C\, e^{\frac{i\,\overrightarrow{p}\,\overrightarrow{r}}{\hbar}} + D\, e^{-\frac{i\,\overrightarrow{p}\,\overrightarrow{r}}{\hbar}} \tag{8.46}$$

8.6 Physical interpretation of solutions to the free Klein-Gordon equation

In order to give a physical meaning to the solutions, we assume

- $e^{-\frac{i\,E}{\hbar}\,t}$ Represents a particle that was created in the past $(-\infty)$ and is traveling towards the future $(+\infty)$.

- $e^{\frac{iE}{\hbar}t}$ Represents a particle created in the future $(+\infty)$ and travels towards the past $(-\infty)$.
- A Represents the probability that the particle being created in the future $(+\infty)$ and traveling towards the past $(-\infty)$.
- B Represents the probability that the particle was created in the past, extending from negative infinity $(-\infty)$, and is now moving towards the future, represented by positive infinity $(+\infty)$.

Therefor, the physical solution is given by

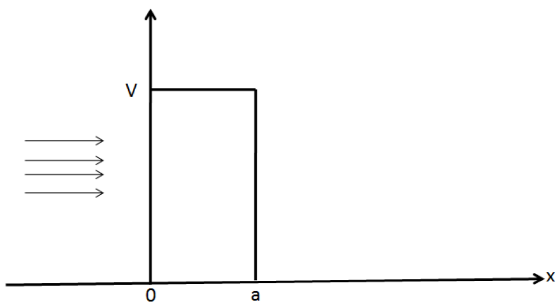
$$f(t) = e^{-\frac{iE}{\hbar}t} \tag{8.47}$$

It signifies the probability that the particle was created in the past, extending from negative infinity, and is now moving towards the future, represented by positive infinity

$$\phi(\overrightarrow{r},t) = f(t)\cdot\psi(\overrightarrow{r}) = e^{-\frac{iE}{\hbar}t}\left(C\,e^{\frac{i\overrightarrow{p}\,\overrightarrow{r}}{\hbar}} + D\,e^{-\frac{i\overrightarrow{p}\,\overrightarrow{r}}{\hbar}}\right) \tag{8.48}$$

Exercice 7 :

The particles with spin 0, charge q, and mass m are approaching from $(+\infty)$ to $(-\infty)$ on a potential barrier of height V and width a. Given that the energy of these particles is given by $E = qV/2$, where $qV > 2mc^2$,



1. Calculate the transmission coefficients T and reflection coefficients R.
2. Calculate the current density J_x in each region.

Indication: Working on one dimension.