

# Relativistic Quantum Waves (Klein-Gordon Equation

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2025-11-14

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# Chapter 1

## Deriving the KG Equation

### 1.1 double deriving

**Definition 1.1.1: Relativity: the mass shell**

$$p \cdot p = (mc)^2 \rightarrow (mc)^2 = \left(\frac{E}{c}\right)^2 - p_x^2 - p_y^2 - p_z^2$$

**Definition 1.1.2: Quantum: energy and momentum operators**

$$\hat{E} = i\hbar \frac{\partial}{\partial t}, \text{ so } \left(\frac{E}{c}\right)^2 \text{ becomes } -\frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2}.$$

$$\hat{p} = -i\hbar \nabla, \text{ so } -p_x^2 \text{ becomes } \hbar^2 \frac{\partial^2}{\partial x^2}.$$

$$\text{likewise, } -p_y^2 \text{ becomes } \hbar^2 \frac{\partial^2}{\partial y^2} \text{ and } -p_z^2 \text{ becomes } \hbar^2 \frac{\partial^2}{\partial z^2}.$$

### 1.2 Plugging in the new values

we can now plugin these into the original equation:

$$\begin{aligned} (mc)^2 &= \left(\frac{E}{c}\right)^2 - p_x^2 - p_y^2 - p_z^2 \\ (mc)^2 &= -\frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2} + \hbar^2 \frac{\partial^2}{\partial x^2} + \hbar^2 \frac{\partial^2}{\partial y^2} + \hbar^2 \frac{\partial^2}{\partial z^2} \\ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 &= 0. \end{aligned}$$

### 1.3 this is the Klein-Gordon Equation!

$$\frac{2}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 = 0 \quad (1.1)$$

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \left(\frac{mc}{\hbar}\right)^2 \right] \psi = 0 \quad (1.2)$$

## 1.4 Replacing with Laplacian

We know that  $-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} = \nabla^2$  -otherwise known as a Laplacian

So the function becomes

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \left( \frac{mc}{\hbar} \right)^2 \right] \psi = 0 \quad (1.3)$$

## 1.5 d'Alembertian

$\square =$  d'Alembertian

We can also rewrite  $\left( \frac{mc}{\hbar} \right)^2$  as  $\mu^2$

**Note:-**

We could also write  $\left( \frac{mc}{\hbar} \right)$  as just  $m$  as in this universe it would become  $(\frac{m \cdot 1}{1})$  which is just the mass but this is the correct way to write it.

So our final equation becomes

$$[\square + \mu^2] \psi = 0 \quad (1.4)$$

## Chapter 2

# Four-momentum Eigenstates

### 2.1 Klein-Gordon Plane Wave

**Definition 2.1.1: Klein-Gorden Plane Wave function**

$$\psi = A \exp(-\frac{i}{\hbar} p \cdot x)$$

$$p = [E/c, \vec{p}], \quad x = [ct, \vec{x}]$$

$$A \in \mathbb{C}, \quad p^0 = \frac{E}{c} 0 \pm \sqrt{|\vec{p}|^2 + m^2 c^2}$$

we can rewrite the original Equation as:

$$\psi = A \exp\left(\frac{i}{\hbar} (\vec{p} \cdot \vec{x} - Et)\right)$$

$$\psi = A \exp\left(\frac{i}{\hbar} \left(\vec{p} \cdot \vec{x} \pm c \sqrt{|\vec{p}|^2 + m^2 c^2 t}\right)\right)$$

### 2.2 Proof that plane waves $\psi = A \exp[-ip \cdot x/\hbar]$ satisfy K.G.

$$\text{rewrite K.G.: } [\square + \mu^2] \psi = 0 \rightarrow \square \psi = -\mu^2 \psi$$

Does d'Alembertian do the same thing as multiplying by  $-\mu^2$ ?

$$\square = \square \left[ \exp\left(-\frac{i}{\hbar} p \cdot x\right) \right] = \square \left[ \exp\left(\frac{i}{\hbar} (\vec{p} \cdot \vec{x} - Et)\right) \right] \quad (2.1)$$

$$\text{Definition of d'Alembertian: } \square = \frac{1}{c^2} \frac{\partial}{\partial t^2} - \nabla^2$$

$$\square = \left[ -\left(\frac{E}{c\hbar}\right) + \left(\frac{|\vec{p}|^2}{\hbar}\right) \right] \exp\left[\frac{i}{\hbar} (\vec{p} \cdot \vec{x} - Et)\right] = -\left(\frac{mc}{\hbar}\right)^2 \psi \quad (2.2)$$

...

# Chapter 3

## Superposition

### 3.1 You can add together many states that solve K.G., and the resulting sum also solves K.G.

Another important concept we have to know about when working with the Klein-Gordon Equation is that any superposition of wave functions that satisfy the Klein-Gordon Equation, also satisfy the Klein-Gordon Equation. That lets us create a complex landscape starting with the simple basis set of functions

Let's say that you have two functions that satisfy the Klein-Gordon Equation, call them  $\psi_1$  and  $\psi_2$

$$[\square + \mu^2] \psi_1 = 0 \quad (3.1)$$

$$[\square + \mu^2] \psi_2 = 0 \quad (3.2)$$

Let's call their sum  $\psi_3$  so

$$\psi_3 = \psi_1 + \psi_2.$$

The question then arises: does  $\psi_3$  satisfy the Klein-Gordon Equation?

Well, yes it does. We can show this with:

$$\begin{aligned} [\square + \mu^2] \psi_3 &= [\square + \mu^2] (\psi_1 + \psi_2) \\ &= [\square + \mu^2] \psi_1 + [\square + \mu^2] \psi_2 = 0 + 0 = 0 \dots \text{also satisfies K.G..} \end{aligned}$$

The following reasoning does not just apply to the sum of two wave functions, but also scaling up a wave function or taking the arbitrary sum over many wave functions. Or even more usefully if you have a basis set of functions that satisfy the Klein-Gordon Equation, then you can make wave functions of that basis set by summing over them with some series of coefficients

Say we write a wavefunction  $\psi$  as a linear combination of  $\{\psi_n\}$

$$\psi = \sum_n C_n \psi_n, \quad C_n \in \mathbb{C} \quad (3.3)$$

Since each basis function in  $\psi_n \in \{\psi_n\}$  satisfies K.G....

$$[\square + \mu^2] \psi_n = 0 \rightarrow [\square + \mu^2] \sum_n C_n \psi_n = 0 \quad (3.4)$$

And that's how we actually use energy and momentum in Eigen-states most of the time.

# Chapter 4

## Group Velocity, and c Speed limit

### 4.1 calculating the group velocity of a Klein-Gordon Wave packet

In order to calculate the group velocity of a Klein-Gordon Wave packet, we first have to calculate something called the **DispersionRelation**.

The **DispersionRelation** is when **angularfrequency**  $\omega$  is written as a function of **angularwavenumber**.

General form of plane wave:

$$\psi = A \exp \left( i \left( \vec{k} \cdot \vec{x} - \omega t \right) \right) \quad (4.1)$$

Klein-Gordon plane wave:

$$\psi = A \exp \left( \frac{i}{\hbar} \left( \vec{p} \cdot \vec{x} \pm c \sqrt{|\vec{p}|^2 + m^2 c^2 t} \right) \right) \quad (4.2)$$

$$\begin{aligned} \omega &= \frac{c}{\hbar} \sqrt{|\vec{p}|^2 + m^2 c^2}, & k &= |\vec{p}| / \hbar \\ |\vec{p}|^2 &= \hbar^2 k^2, & \rightarrow \omega &= \sqrt{(kc)^2 + \left( \frac{mc^2}{\hbar} \right)^2} \end{aligned}$$

### 4.2 Finding the group relation

Now we have the Dispersion Relation:  $\omega = \sqrt{(kc)^2 + \left( \frac{mc^2}{\hbar} \right)^2}$

The group velocity is then:  $v_g = \frac{d\omega}{dk}$

$$v_g = \frac{d}{dk} \left[ \sqrt{(kc)^2 + (mc^2/\hbar)^2} \right] \quad (4.3)$$

with  $k = |\vec{p}| / \hbar$  in mind:

$$v_g = \frac{kc}{\sqrt{k^2 + (mc/\hbar)^2}} \rightarrow v_g = \frac{c |\vec{p}|}{\sqrt{|\vec{p}|^2 + (mc)^2}} \quad (4.4)$$

Playing around with the Klein-Gordon equation, we have found a speed limit: the speed of light!

Massive particle: can only approach  $c$  as momentum increases, can never reach  $c$ .

Massless particle: always travels at  $c$ , regardless of momentum. – Light always travels at  $c$  in all reference frames!

# Chapter 5

## Fourier transform and antimatter

### 5.1 Complex Coefficients on the Mass Shell

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \exp\left[-\frac{i}{\hbar} p \cdot x\right] dp \quad (5.1)$$

- wavefunction in spacetime
- Normalization constant
- Add up eigenstate for each  $p$ , weighted  $\phi(p)$
- Momentum-space wavefunction
- $p$ -eigenstate

### 5.2 The Two Halves of the Mass Shell

There is a one-to-one connection between all possible wavefunctions that satisfy the Klein-Gordon equation in spacetime and all possible ways of decorating the mass shell with complex numbers.

**The critical insight:** You need *both halves* of the mass shell to have a complete basis set for Fourier transforms from momentum space to position space.

Recall from the plane wave solution that:

$$p^0 = \frac{E}{c} = \pm \sqrt{|\vec{p}|^2 + m^2 c^2} \quad (5.2)$$

This  $\pm$  sign gives us two branches:

- **Positive energy:**  $E = +\sqrt{p^2 c^2 + m^2 c^4}$  (normal particles)
- **Negative energy:**  $E = -\sqrt{p^2 c^2 + m^2 c^4}$  (antimatter!)

### 5.3 Dirac's Critique: The Fatal Flaws of Klein-Gordon

Dirac identified two deeply connected problems with the Klein-Gordon equation that made it unsuitable as a single-particle quantum theory.

### 5.3.1 Problem 1: Second-Order in Time

The Klein-Gordon equation is **second-order in time**.

Compare the time derivatives:

$$\begin{aligned} \text{Schrödinger: } & i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \quad (\text{first-order in time}) \\ \text{Klein-Gordon: } & \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi + \left(\frac{mc}{\hbar}\right)^2 \psi = 0 \quad (\text{second-order in time}) \end{aligned}$$

Being second-order in time allows both positive and negative energy solutions and treats space and time on equal footing (manifestly relativistic). However, it creates a serious problem.

**Too much freedom!** Just like classical mechanics needs position AND velocity for second-order equations, Klein-Gordon requires *two* initial conditions:

- The wavefunction:  $\psi(x, 0)$

- The time derivative:  $\left. \frac{\partial \psi}{\partial t} \right|_{t=0}$

In quantum mechanics, the state should be completely determined by  $\psi(x, 0)$  alone. Having  $\partial\psi/\partial t$  as an independent initial condition violates this fundamental principle.

### 5.3.2 Problem 2: Negative Probability Density

This "too much freedom" problem directly causes the negative probability issue.

For Schrödinger, the probability density is simple:

$$\rho = |\psi|^2 = \psi^* \psi \geq 0 \quad (\text{always positive!}) \quad (5.3)$$

For Klein-Gordon, deriving the probability density from the continuity equation gives:

$$\rho = \frac{i\hbar}{2mc^2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \quad (5.4)$$

**This depends on both  $\psi$  and  $\partial\psi/\partial t$ !** Since  $\partial\psi/\partial t$  is an independent degree of freedom (Problem 1), we can choose it to make  $\rho$  negative. Negative probabilities are physically nonsensical.

**The connection:** The negative probability problem exists *because* the equation is second-order in time. These aren't separate issues — they're two sides of the same coin.

### 5.3.3 Dirac's Solution

Dirac wanted the impossible:

1. **First-order in time** (like Schrödinger) — needs only  $\psi(x, 0)$ , no extra freedom
2. **Relativistically correct** — treats energy and momentum on equal footing
3. **Positive definite probability** —  $\rho \geq 0$  always

This seemingly impossible requirement led Dirac to discover the **Dirac equation**, which is first-order in *both* time and space. The price? The wavefunction becomes a multi-component spinor, and quantum mechanical spin emerges naturally!

## 5.4 Reinterpreting Negative Energy: Feynman-Stueckelberg

While Dirac's equation solved the problems above, the negative energy solutions still appear. But there's a beautiful reinterpretation that doesn't require "negative energy" at all.

Recall the energy operator:

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (5.5)$$

**Shift your perspective:** Instead of thinking about negative energy, reinterpret what  $-\hat{E}$  means:

$$-\hat{E} = -i\hbar \frac{\partial}{\partial t} \quad (5.6)$$

Negative energy??  $\longrightarrow$  Time reversal!

A *negative energy* particle moving *forward in time* is mathematically equivalent to a *positive energy* antiparticle moving *backward in time*.

This is the **Feynman-Stueckelberg interpretation**:

- Particles: positive energy, moving forward in time
- Antiparticles: positive energy, moving backward in time (which *looks like* negative energy forward in time)

When an electron and positron annihilate, you can picture the positron as an electron that reversed its direction in time!

**The Resolution:** The negative energy solutions represent *antimatter*. When you include both halves of the mass shell, you're accounting for both particles and antiparticles. Klein-Gordon isn't a single-particle theory — it's fundamentally a quantum field theory equation.