Relativistic Quantum Waves (Klein-Gordon Equation

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Contents

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:

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

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

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

1.3 this is the Klein-Gordon Equation!

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

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

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

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

1.5 d'Alembertian

$\square =$ d'Alembertian
We can also rewrite $\left(\frac{mc}{\hbar}\right)^2$ as μ^2

Note:-

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

So our final equation becomes

$$\left[\square + \mu^2\right]\psi = 0 \tag{1.4}$$

Chapter 2

Four-momentum Eigenstates

2.1 Klein-Gordon Plane Wave

Definition 2.1.1: Klein-Gorden Plane Wave function

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

$$\begin{aligned} p = \left[E/c, \vec{p}\right], \qquad & x = \left[ct, \vec{x}\right] \\ A \in \mathbb{C}, \qquad & p^0 = \frac{E}{c} 0 \pm \sqrt{\left|\vec{p}\right|^2 + m^2 c^2} \end{aligned}$$

we can rewrite the original Equation as:

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

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

rewrite K.G.: $\left[\Box + \mu^3\right] \psi = 0 \rightarrow \Box\psi = -\mu^2 \psi$

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

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

Definition of d'Alembertian: $\Box = \dfrac{1}{c^2} \dfrac{\partial}{\partial t^2} - \nabla^2$

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

...

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 ψ_1 and ψ_2

$$\left[\Box + \mu^2\right] \psi_1 = 0 \tag{3.1}$$

$$\left[\Box + \mu^2\right] \psi_2 = 0 \tag{3.2}$$

Let's call their sum ψ_3 so

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

The question then arises: does ψ_3 satisfy the Klein-Gordon Equation?
Well, yes it does. We can show this with:

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

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 ψ as a linear combination of $\left\{\psi_n\right\}$

$$\psi = \sum_n C_n \psi_n, \qquad C_n \in \mathbb{C} \tag{3.3}$$

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

$$\left[\Box + \mu^2\right] \psi_n = 0 \rightarrow \left[\Box + \mu^2\right] \sum_n C_n \psi_n = 0 \tag{3.4}$$

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**ω is written as a function of **angularwavenumber**.

General form of plane wave:

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

Klein-Gordon plane wave:

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

$$\omega = \frac{c}{\hbar}\sqrt{\left|\vec{p}\right|^2 + m^2c^2}, \qquad k = \left|\vec{p}\right|/\hbar$$

$$\left|\vec{p}\right|^2 = \hbar^2 k^2, \qquad \rightarrow \omega = \sqrt{(kc)^2 + \left(\frac{mc^2}{\hbar}\right)^2}$$

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: $v_g = \frac{d\omega}{dk}$

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

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

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

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

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

- 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:

$$p^0 = \frac{E}{c} = \pm\sqrt{\left|\vec{p}\right|^2 + m^2c^2} \tag{5.2}$$

This $\pm$ sign gives us two branches:

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

5.2.1 The Negative Energy Problem

The Klein-Gordon equation has a serious problem compared to the Schrödinger equation.

For Schrödinger, the probability density is: $\rho = |\psi|^2 = \psi^*\psi \geqslant 0 \quad$ (always positive!)

But for Klein-Gordon, the probability density is:

$$\rho = \frac{i\hbar}{2mc^2}\left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}\right) \tag{5.3}$$

This can be **negative**! This is a major problem because probability cannot be negative.

The Resolution: The negative energy solutions are not unphysical errors — they represent *antimatter*. When you include both halves of the mass shell, you're accounting for both particles and their antiparticles. This is why Klein-Gordon is fundamentally a quantum field theory equation, not a single-particle quantum mechanics equation.

5.2.2 Feynman-Stueckelberg Interpretation: Time Reversal

There's a beautiful way to reinterpret negative energy solutions that doesn't require "negative energy" at all.

Recall the energy operator:

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{5.4}$$

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

$$-\hat{E} = -i\hbar\frac{\partial}{\partial t} \quad \longrightarrow \quad -\hat{E} = -i\hbar\frac{\partial}{\partial t} \tag{5.5}$$

$$\text{Negative energy??} \quad \longrightarrow \quad \text{Time reversal!}$$

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!

5.3 Dirac's Critique: Second-Order in Time Problem

The Klein-Gordon equation has another fundamental issue that bothered Dirac: it is **second-order in time**.

Compare the time derivatives:

$$\text{Schrödinger:} \quad i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \quad \text{(first-order in time)}$$

$$\text{Klein-Gordon:} \quad \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2\psi = 0 \quad \text{(second-order in time)}$$

5.3.1 What Does Second-Order Unlock?

Being second-order in time is what allows the Klein-Gordon equation to have both positive and negative energy solutions. It treats space and time on equal footing (both second derivatives), making it manifestly relativistic.

However, this creates a serious conceptual problem.

5.3.2 Too Much Freedom?

In classical mechanics, a second-order differential equation requires *two* initial conditions:

- Position: $x(0)$

- Velocity: $\left.\frac{dx}{dt}\right|_{t=0}$

Similarly, the Klein-Gordon equation (being second-order in time) requires *two* initial conditions:

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

This is too much freedom! In quantum mechanics, we want to specify the *state* of the system at one instant in time. The state should be completely determined by the wavefunction $\psi(x, 0)$ alone, not by its time derivative.

The first derivative in time $\partial\psi/\partial t$ becomes an independent initial condition — we can choose it freely. This means the Klein-Gordon equation doesn't have a unique time evolution from a given initial wavefunction, which violates a fundamental principle of quantum mechanics.

5.3.3 Dirac's Solution

This was one of Dirac's fundamental critiques of the Klein-Gordon equation. He wanted:

1. **First-order in time** (like Schrödinger) — more restrictive, needs only $\psi(x, 0)$
2. **Relativistically correct** (treating space and time properly)

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, introducing the concept of quantum mechanical spin!