The Klein-Gordon equation and the meson π^-

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Abstract

The study of the free motion of the meson π^- through the equation of Klein-Gordon, leads to its antiparticle i.e. the meson π^+.

1 The Klein-Gordon equation

Let us remember that the quantum-mechanical state of a non-relativistic particle of mass m and spin 0 is a solution of the Schrödinger equation which we write here in operational form:

$$\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t} \tag{1}$$

where

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}) \tag{2}$$

is the Hamiltonian operator, while $\psi(\mathbf{x}, t)$ is the wave function of the particle. Let us quickly recall the representation of the various operators in the coordinate base [1]

$$\hat{\mathbf{p}} \doteq -i\hbar\nabla \Longrightarrow \hat{H} \doteq -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$$

so we find the well-known form of the Scrhödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi = i\hbar\frac{\partial \psi}{\partial t} \tag{3}$$

In l926 Klein, Gordon and Fok (and perhaps even Schrödinger himself before writing his famous equation (3)) used the following device (E is energy):

$$E \to i\hbar\frac{\partial}{\partial t}, \quad p \to -i\hbar\nabla \tag{4}$$

where for simplicity we are considering the one-dimensional case. From relativistic mechanics [3]:

$$E^2 = m^2c^4 + c^2p^2$$

It follows that substitution (4) returns

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

The generalization to three-dimensional motion is immediate:

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \left(\frac{mc}{\hbar}\right)^2\psi = 0 \tag{5}$$

known as **Klein–Gordon equation**. A notable difference from that of Schrödinger is that the K-G is of the second order in the time derivative. And this will present probl

After some manipulation, we arrive at the continuity equation for magnitude

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

Precisely:

$$\frac{\partial\rho}{\partial t}+\operatorname{div}\mathbf{j}=0 \tag{6}$$

where

$$\mathbf{j}(\mathbf{x},t)=\frac{\hbar}{2im}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right) \tag{7}$$

We are tempted to call ρ ≪probability density≫, but the presence of the second derivative with respect to time in the K-G leads to an inconsistency. Precisely, since the second order equation "resembles" the D'Alembert one, we have that a Cauchy problem is characterized by initial conditions (with obvious meaning of the symbols):

$$\psi(\mathbf{x},0)=\varphi(\mathbf{x}),\quad \left.\frac{\partial\psi}{\partial t}\right|_{(\mathbf{x},0)}=\chi(\mathbf{x})$$

where functions are assigned arbitrarily. This implies that the quantity ρ is not positive definite, so it is not a probability density. A possible re-interpretation consists in redefining:

$$\begin{aligned}\rho(\mathbf{x},t)&=\frac{iq\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)\\ \mathbf{j}(\mathbf{x},t)&=\frac{q\hbar}{2im}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)\end{aligned} \tag{8}$$

being q the electric charge (possibly zero) of the particle. We are interested in solutions of the monochromatic plane wave type which, as is known, are quantum states with a defined momentum value. Without violating generality, let's consider the one-dimensional case:

$$\frac{\partial^2\psi}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}-\left(\frac{mc}{\hbar}\right)^2\psi=0 \tag{9}$$

We are looking for solutions like this

$$\psi(x,t)=Ae^{i(kx-\omega t)} \tag{10}$$

After simple steps:

$$\omega^2=c^2\left[k^2+\left(\frac{mc}{\hbar}\right)^2\right]$$

Multiplying the first and second members by Planck's reduced constant and remembering the relationship between pulsation and energy, and between wave number and impulse, we have

$$E^2=c^2p^2+m^2c^4,$$

that is, exactly what is expected. To remove ambiguity about the sign, we define

$$E_P\overset{def}{=}+\sqrt{m^2c^4+c^2p^2} \tag{11}$$

so $E=\pm E_P$. It follows that the solutions (10) are written $\psi_\pm(x,t)=Ae^{\frac{i}{\hbar}(px\mp E_Pt)}$ or in the form more compact:

$$\psi_\lambda(x,t)=Ae^{\frac{i}{\hbar}(px-\lambda E_Pt)},\quad \lambda=\pm1 \tag{12}$$

Here an interpretative problem arises since we still have two progressive plane waves, but one of the two has a "negative frequency"; precisely

$$\lambda = -1 \Longrightarrow \psi_- (x,t) = Ae^{i(kx-(-\omega)t)} \text{ dove } -\omega = -\frac{E_p}{\hbar}$$

which describes a progressive plane wave with frequency $-\omega$. Replacing the (12) in the first of the (8)

$$\rho_\lambda (x,t) = \frac{\lambda q E_P}{mc^2} A^2 \tag{13}$$

where we have redefined the electric charge as $q = e$ where e is the absolute value of the charge of the electron. We can then interpret $\psi_+ (x,t)$ as the wave function of a relativistic free particle of momentum p and electric charge q, while $\psi_- (x,t)$ is the wave function of a relativistic free particle of momentum p and electric charge $-q$.

2 Covariant form of the Klein-Gordon equation

Since the Klein-Gordon equation is the relativistic extension of the Schrödinger equation for a particle of spin 0, we must write it in four-dimensional notation. For this purpose, we recall that the generic point-event of the spacetime of Special Relativity is determined by the 4-vector $x^\mu = (x^0, x^1, x^2, x^3)$ where $x^{(0)} = ct$ is the time coordinate, while (x^1, x^2, x^3) are the spatial coordinates which in many cases coincide with the usual Cartesian coordinates(x, y, z). Here we have a metric tensor

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

and therefore an element of "distance":

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = c^2 dt - (dx)^2 - (dy)^2 - (dz)^2$$

which is manifestly invariant under Lorentz transformations. The 4-momentum of a particle of mass m is defined by the following 4-vector:

$$p^\mu = \left(\frac{E}{c}, \mathbf{p} \right)$$

being $\mathbf{p} = (p^1, p^2, p^3)$ the usual 3-momentum, while E is the energy

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

Performing the scalar product or the contraction of the 4-impulse vector:

$$p^\mu p_\mu = \frac{E^2}{c^2} - \mathbf{p}^2 = m^2 c^2$$

Given this, we need to write the differential equation

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \left(\frac{mc}{\hbar} \right)^2 \psi = 0 \tag{14}$$

in 4-dimensional notation. Let's remember the 4-gradient operator:

$$\partial^\mu = \frac{\partial}{\partial x_\mu} = g^{\mu\nu} \frac{\partial}{\partial x_\nu},$$

where $g^{\mu\nu}$ is the inverse metric tensor. We have

$$\frac{\partial}{\partial x^{\mu}} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}\right) = \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right) \Longrightarrow \partial^{\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right)$$

It follows

$$\partial^{\mu}\partial_{\mu} = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 = -\Box$$

Incidentally, passing from the individual physical quantities to the respective Hermitian operators:

$$\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla \Longrightarrow p^{\mu} \to \hat{p}^{\mu} = -i\hbar\partial^{\mu}$$

Ultimately, in 4-dimensional notation the Klein-Gordon equation is written:

$$(\partial^{\mu}\partial_{\mu})\,\psi = -\left(\frac{mc}{\hbar}\right)^2\psi$$

which is manifestly covariant.

3 Integration of the Klein-Gordon equation

After examining the covariant writing of the Klein - Gordon equation, let's rewrite it in three-dimensional notation:

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = \left(\frac{mc}{\hbar}\right)^2\psi \tag{15}$$

Let them be

$$\varphi, \chi \mid \psi = \varphi + \chi, \quad i\hbar\frac{\partial\psi}{\partial t} = mc^2(\varphi - \chi)$$

It follows

$$\nabla^2(\varphi+\chi) - \frac{1}{c^2}\frac{\partial}{\partial t}\left[-\frac{i}{\hbar}mc^2(\varphi-\chi) - \frac{m^2c^2}{\hbar^2}(\varphi+\chi)\right] = 0$$
$$\Longrightarrow \nabla^2\varphi + \nabla^2\chi + \frac{i}{\hbar}m\left(\frac{\partial\varphi}{\partial t} - \frac{\partial\chi}{\partial t}\right) - \frac{m^2c^2}{\hbar^2}\varphi - \frac{m^2c^2}{\hbar^2}\chi = 0$$
$$\Longrightarrow \left[\frac{\hbar^2}{2}\nabla^2(\varphi+\chi) - m^2c^2\varphi + i\hbar m\frac{\partial\varphi}{\partial t}\right] - \left[-\frac{\hbar^2}{2}\nabla^2(\varphi+\chi) + i\hbar m\frac{\partial\chi}{\partial t} + m^2c^2\chi\right] = 0$$

It is clear that the terms in brackets must cancel identically, obtaining:

$$\begin{cases} i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2(\varphi+\chi) + mc^2\varphi \\ i\hbar\frac{\partial\chi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2(\varphi+\chi) - mc^2\chi \end{cases} \tag{16}$$

which is a system of two differential equations of the Schrödinger type.

4 Operational form of the Klein-Gordon equation

The mathematical device used in the previous number returns the sensational advantage of reducing the order of the Klein-Gordon differential equation in the time derivative by one unit (reducing it to a Schrödinger equation). The price you pay is the integration of a system of coupled differential equations. The particular shape of this system suggests a matrix writing of the same. To do this, we define the column vector

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{17}$$

whose elements are the unknown functions that appear in the aforementioned system that we rewrite here:

$$\begin{cases} i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\left(\varphi+\chi\right) + mc^2\varphi \\ i\hbar\frac{\partial\chi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\left(\varphi+\chi\right) - mc^2\chi \end{cases} \tag{18}$$

Let's write a Schrödinger-type equation

$$\hat{X}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{19}$$

where

$$\hat{X} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix}$$

whose matrix elements are second-order differential operators acting on the elements of the Hilbert space $L^2\left(\mathbb{R}^3\right)$. Expliciting the product rows by columns, we obtain:

$$\begin{cases} X_{11}\varphi + X_{12}\chi = i\hbar\frac{\partial\varphi}{\partial t} \\ X_{21}\varphi + X_{22}\chi = i\hbar\frac{\partial\chi}{\partial t} \end{cases}$$

from which

$$\begin{aligned} X_{11} &= -\frac{\hbar^2}{2m}\nabla^2 + mc^2, \;\; X_{12} = -\frac{\hbar^2}{2m}\nabla^2 \\ X_{21} &= \frac{\hbar^2}{2m}\nabla^2, \;\; X_{22} = \frac{\hbar^2}{2m}\nabla^2 - mc^2 \end{aligned} \tag{20}$$

To separate matrices by the differential operator nabla, we write

$$\hat{X} = -\frac{\hbar^2}{2m}Y\nabla^2 + mc^2 Z,$$

where Y, Z are matrices (to be determined) of order 2 on the complex field. One possible determination is

$$Y = \tau_3 + i\tau_2, \;\; Z = \tau_3$$

having introduced the matrices:

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \;\; \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \;\; \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{21}$$

which verify the following properties:

$$\tau_k^2 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\tau_k\tau_l = -\tau_l\tau_k = i\tau_m, \quad i = 1,2,3 \;\text{ in ordine ciclico}$$

We conclude that the operational form of the Klein - Gordon equation is:

$$\hat{H}_f\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{22}$$

where the Hamiltonian operator is

$$\hat{H}_f = -\frac{\hbar^2}{2m}\left(\tau_3 + i\tau_2\right)\nabla^2 + mc^2\tau_3 \tag{23}$$

For a physical interpretation of the functions that make up Ψ, we take the electric charge density and the corresponding current density:

$$\begin{aligned}\rho\left(\mathbf{x},t\right) &= \frac{iq\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)\\ \mathbf{j}\left(\mathbf{x},t\right) &= \frac{q\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\end{aligned}$$

It follows

$$\rho = \frac{iq\hbar}{2mc^2}\left[\frac{mc^2}{i\hbar}\left(\varphi^* + \chi^*\right)\left(\varphi - \chi\right) + \frac{mc^2}{i\hbar}\left(\varphi + \chi\right)\left(\varphi^* - \chi^*\right)\right]$$

$$\rho = q\left(\varphi\varphi^* - \chi\chi^*\right) \tag{24}$$

The obvious result

$$\left(\begin{array}{cc}\varphi^* & \chi^*\end{array}\right)\underbrace{\left(\begin{array}{cc}1 & 0\\ 0 & -1\end{array}\right)}_{=\tau_3}\left(\begin{array}{c}\varphi\\ \chi\end{array}\right) = \varphi\varphi^* - \chi\chi^*$$

allows us to express the charge density as

$$\rho = q\Psi^\dagger\tau_3\Psi$$

being

$$\Psi^\dagger = \left(\begin{array}{cc}\varphi^* & \chi^*\end{array}\right)$$

the conjugate Hermitian function of Ψ. The electric charge in a volume of physical space represented by a regular domain Ω, is

$$Q_\Omega\left(t\right) = \int_\Omega \rho\left(\mathbf{x},t\right)d^3x = q\int_\Omega\left(\varphi\varphi^* - \chi\chi^*\right)d^3x$$

Density and current are related by the continuity equation

$$\frac{\partial\rho}{\partial t} + \operatorname{div}\mathbf{j} = 0 \tag{25}$$

cwhich expresses the conservation of electric charge. Integrating over all physical space manifestly results

$$\frac{dQ}{dt} = 0, \qquad (Q = \int_{\mathbb{R}^3}\rho d^3x) \tag{26}$$

with the normalization condition:

$$\int_{\mathbb{R}^3}\rho d^3x = \pm e$$

i.e.

$$\int_{\mathbb{R}^3}\Psi^\dagger\tau_3\Psi d^3x = \begin{cases}+1, & \text{if } +e\\ -1, & \text{if } -e\end{cases} \tag{27}$$

5 Free motion. Particle and antiparticle

The free motion of a particle is described by a «wave function»

$$\Psi(\mathbf{x},t) = \begin{pmatrix} \varphi(\mathbf{x},t) \\ \chi(\mathbf{x},t) \end{pmatrix} \tag{28}$$

where

$$\varphi(\mathbf{x},t) = \varphi_0 e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-\varepsilon t)}; \quad \chi(\mathbf{x},t) = \chi_0 e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-\varepsilon t)} \tag{29}$$

being φ_0, χ_0 constant quantities. So

$$\Psi(\mathbf{x},t) = \begin{pmatrix} \varphi_0 \\ \chi_0 \end{pmatrix} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-\varepsilon t)} \tag{30}$$

assuming that (30) is a solution of (22) we obtain the system of equations:

$$\begin{cases} (\varepsilon - mc^2)\,\varphi_0 = \frac{p^2}{2m}(\varphi_0 + \chi_0) \\ (\varepsilon + mc^2)\,\chi_0 = -\frac{p^2}{2m}(\varphi_0 + \chi_0) \end{cases} \tag{31}$$

It follows

$$\exists!\,(\varphi_0, \chi_0) \neq (0,0) \iff \varepsilon = \pm E_P \quad \text{where } E_P = +\sqrt{m^2c^4 + c^2p^2}$$

So

$$\Psi_{(+)}(\mathbf{x},t) = \begin{pmatrix} \varphi_{0(+)} \\ \chi_{0(+)} \end{pmatrix} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-E_P t)} \tag{32}$$

$$\varphi_{0(+)} = \frac{E_P + mc^2}{2\sqrt{mc^2 E_P}}, \quad \chi_{0(+)} = \frac{mc^2 - E_P}{2\sqrt{mc^2 E_P}}$$

and

$$\Psi_{(-)}(\mathbf{x},t) = \begin{pmatrix} \varphi_{0(-)} \\ \chi_{0(-)} \end{pmatrix} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}+E_P t)} \tag{33}$$

$$\varphi_{0(+)} = \frac{E_P + mc^2}{2\sqrt{mc^2 E_P}}, \quad \chi_{0(+)} = \frac{mc^2 - E_P}{2\sqrt{mc^2 E_P}}$$

To write the normalization condition, we first observe that the constant quantities φ_0, χ_0 are dimensionless. Since a wave function has the dimensions of $V^{-1/2}$ where V V is a volume, we must multiply by a constant quantity A having this dimension. To normalize it is however convenient to refer to the motion in a region Ω of volume V, so

$$\Psi_{(\pm)}(\mathbf{x},t) = V^{-1/2} \begin{pmatrix} \varphi_{0(+)} \\ \chi_{0(+)} \end{pmatrix} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}\mp E_P t)} \tag{34}$$

The normalization condition immediately follows

$$\varphi_{0(\pm)}\varphi_{0(\pm)} - \chi_{0(\pm)}\,\chi_{0(\pm)} = \pm 1 \tag{35}$$

We refer to the motion of the positively charged particle:

$$\Psi_{(+)}(\mathbf{x},t) = \begin{pmatrix} \varphi_{0(+)} \\ \chi_{0(+)} \end{pmatrix} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-E_P t)} = \begin{pmatrix} \varphi_{(+)}(\mathbf{x},t) \\ \chi_{(+)}(\mathbf{x},t) \end{pmatrix} \tag{36}$$

So let's define

$$\Psi_c(\mathbf{x},t) = \begin{pmatrix} \chi^*_{(+)}(\mathbf{x},t) \\ \varphi^*_{(+)}(\mathbf{x},t) \end{pmatrix}$$
$$= \begin{pmatrix} \chi_{0(+)} \\ \varphi_{0(+)} \end{pmatrix} e^{\frac{i}{\hbar}[(-\mathbf{p})\cdot\mathbf{x}+E_P t]}$$

so Ψ_c describes the motion of a particle with negative charge and momentum $-\mathbf{p}$. The reverse is also true:

$$\Psi_{(-)} = \begin{pmatrix} \varphi_{(-)} \\ \chi_{(-)} \end{pmatrix} \rightarrow \Psi_c = \begin{pmatrix} \chi^*_{(-)} \\ \varphi^*_{(-)} \end{pmatrix} \quad (37)$$

Here Ψ_c describes the motion of a positively charged particle. We conclude that there is a solution $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ the solution corresponds uniquely $\Psi_c = \begin{pmatrix} \chi^* \\ \varphi^* \end{pmatrix}$ which is called the solution of the *conjugated charge* relative to Ψ. Note that

$$\Psi_c = \tau_1 \Psi \quad (38)$$

Definition 1 *If the relativistic motion of a particle of mass m and spins $= 0$ is described by the "wave function"*

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix},$$

the particle described by the conjugate charge function $\Psi_c = \tau_1 \Psi$, it's called **antiparticle**.

Example 2 *The meson π^- has zero spin and charge $q = -e$. It follows that the meson π^+ is the antiparticle.*

Definition 3 *The transformation*

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \longrightarrow \Psi_c = \begin{pmatrix} \chi^* \\ \varphi^* \end{pmatrix} \quad (39)$$

is called **conjugation particle – antiparticle**. *The (39) transforms particles into antiparticles and vice versa. If the state of motion is invariant with respect to (39), the particle is said to be* **effectively neutral**.

Example 4 *The neutron and neutrino are electrically neutral particles but not actually neutral. The photon is an electrically neutral and effectively neutral particle.*

References

[1] Sakurai J.J., *Modern Quantum Mechanics*.

[2] Davydov A.S., *Meccanica Quantistica*. Editori Riuniti.

[3] Landau L. D. Lifsits M.L. *Fisica Teorica 2. Teoria dei campi*. Editori Riuniti.