3 Klein-Gordon Equation

In non-relativistic mechanics, the energy for a free particle is

$$E = \frac{p^2}{2m}. \tag{35}$$

To get quantum mechanics, we make the following substitutions:

$$E \to i\hbar\frac{\partial}{\partial t}, \quad \boldsymbol{p} \to -i\hbar\boldsymbol{\nabla}, \tag{36}$$

and the Schrödinger equation for a free particle is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{37}$$

In relativistic mechanics, the energy of a free particle is

$$E = \sqrt{p^2c^2 + m^2c^4}. \tag{38}$$

Making the same substitution we obtain

$$\sqrt{-\hbar^2c^2\nabla^2 + m^2c^2}\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{39}$$

It's difficult to interprete the operator on the left hand side, so instead we try

$$\begin{aligned} E^2 &= p^2c^2 + m^2c^4 && (40)\\ \Rightarrow \left(i\hbar\frac{\partial}{\partial t}\right)^2\Psi &= -\hbar^2c^2\nabla^2 + m^2c^4\Psi, && (41)\\ \text{or } \frac{1}{c^2}\left(\frac{\partial}{\partial t}\right)^2\Psi - \nabla^2\Psi &\equiv \Box\Psi = -\frac{m^2c^2}{\hbar^2}\Psi, && (42) \end{aligned}$$

where

$$\Box = \frac{1}{c^2}\left(\frac{\partial}{\partial t}\right)^2 - \nabla^2 = \partial_\mu\partial^\mu. \tag{43}$$

Plane-wave solutions are readily found by inspection,

$$\Psi = \frac{1}{\sqrt{V}}\exp\left(\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}\right)\exp\left(-\frac{i}{\hbar}Et\right), \tag{44}$$

where $E^2 = p^2c^2 + m^2c^4$ and thus $E = \pm\sqrt{p^2c^2 + m^2c^4}$. Note that there is a negative energy solution as well as a positive energy solution for each value of $\boldsymbol{p}$. Naïvely one should just discard the negative energy solution. For a free particle in a positive energy state, there is no mechanism for it to make a transition to the negative energy state. However, if there is some external potential, the Klein-Gordon equation is then altered by the usual replacements,

$$E \to E - e\phi, \quad \boldsymbol{p} \to \boldsymbol{p} - \frac{e}{c}\boldsymbol{A}, \tag{45}$$

$$(i\hbar\partial_t - e\phi)^2\Psi = c^2(-i\hbar\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A})^2\Psi + m^2c^4\Psi. \tag{46}$$

The solution Ψ can always be expressed as a superposition of free particle solutions, provided that the latter form a **complete set**. They from a complete set only if the negative energy components are retained, so they cannot be simply discarded.

Recall the probability density and current in Schrödinger equation. If we multiply the Schrödinger equation by Ψ^* on the left and multiply the conjugate of the Schrödinger equation by Ψ, and then take the difference, we obtain

$$\begin{aligned} -\frac{\hbar^2}{2m}(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*) &= i\hbar(\Psi^*\dot{\Psi} + \Psi\dot{\Psi}^*) \\ \Rightarrow -\frac{\hbar^2}{2m}\boldsymbol{\nabla}(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*) &= i\hbar\frac{\partial}{\partial t}(\Psi^*\Psi) \end{aligned} \tag{47}$$

Using $\rho_s = \Psi^*\Psi$, $\boldsymbol{j}_s = \frac{\hbar}{2mi}(\Psi^*\boldsymbol{\nabla}\Psi - \Psi\boldsymbol{\nabla}\Psi^*)$, we then obtain the equation of continuity,

$$\frac{\partial\rho_s}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{j}_s = 0 \tag{48}$$

Now we can carry out the same procedure for the free-particle Klein-Gordon equation:

$$\begin{aligned} \Psi^*\Box\Psi &= -\frac{m^2c^2}{\hbar}\Psi^*\Psi \\ \Psi\Box\Psi^* &= -\frac{m^2c^2}{\hbar}\Psi\Psi^* \end{aligned} \tag{49}$$

Taking the difference, we obtain

$$\Psi^*\Box\Psi - \Psi\Box\Psi^* = \partial_\mu(\Psi^*\partial^\mu\Psi - |psi\partial^\mu\Psi^*) = 0. \tag{50}$$

This suggests that we can define a probability 4-current,

$$j^\mu = \alpha(\Psi\partial^\mu\Psi - \Psi\partial^\mu\Psi^*), \quad \text{where } \alpha \text{ is a constant} \tag{51}$$

and it's conserved, $\partial_\mu j^\mu = 0$, $j^\mu = (j^0, \boldsymbol{j})$. To make $\boldsymbol{j}$ agree with $\boldsymbol{j}_s$, α is chosen to be $\alpha = -\frac{\hbar}{2mi}$. So,

$$\rho = \frac{j^0}{c} = \frac{i\hbar}{2mc^2}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right). \tag{52}$$

ρ does reduce to $\rho_s = \Psi^*\Psi$ in the non-relativistic limit. However, ρ is not positive -definite and hence can not describe a probability density for a single particle.

Pauli and Weisskopf in 1934 showed that Klein-Gordon equation describes a spin-0 (scalar) field. ρ and $\boldsymbol{j}$ are interpreted as charge and current density of the particles in the field.