Chapter 2

Lorentz-invariant Wave Equations

In this chapter we introduce Lorentz-invariant wave equations which are defined as follows: if a wave function satisfies a certain equation in one frame, then when the wave function is transformed to another frame (i.e. 'viewed' in that frame), it satisfies the same form of equation in terms of the coordinates in the latter frame. We then attempt to construct such equation by applying the standard correspondence between energy-momentum and the differential operators $(i\partial_0, -i\vec{\nabla})$ to the relativistic relation $E^2 - \vec{P}^2 = m^2$, which leads us to the Klein-Gordon equation. The probability current is constructed from the wave function such that it is conserved. We will then see that if we adhere to the standard interpretations of energy and probability, it has solutions with negative energy and negative probability. We start this chapter by examining what is meant by energy and probability.

2.1 Energy and momentum

In non-relativistic quantum mechanics, the operators for energy and momentum are given by

$$E:\ i\frac{\partial}{\partial t}\,, \qquad \vec{P}:\ -i\vec{\nabla}\,. \tag{2.1}$$

Thus, in general, a wave function which is an eigenfunction of given values of energy-momentum $(E, \vec{P})$ has the plane-wave form

$$\phi(t, \vec{x}) = C(E, \vec{P})e^{-i(Et - \vec{P}\cdot\vec{x})}, \tag{2.2}$$

where the constant coefficient $C(E, \vec{P})$ in general can have multiple components [which will make $\phi(t, \vec{x})$ multiple-component] and can depend on $(E, \vec{P})$. It clearly gives the desired eigenvalues for energy-momentum:

$$\left(i\frac{\partial}{\partial t}\right)\phi = E\phi\,, \qquad \left(-i\vec{\nabla}\right)\phi = \vec{P}\phi\,. \tag{2.3}$$

Namely, the wave length at a fixed time gives the momentum and the oscillation frequency at a fixed position gives the energy. According to the definition (2.1), the sense of the phase rotation with respect to time gives the sign of energy:

$$\phi \sim e^{-i|E|t} : \text{positive energy}, \quad \phi \sim e^{+i|E|t} : \text{negative energy}\,. \tag{2.4}$$

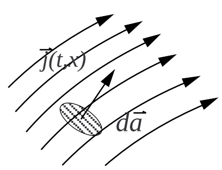
2.2 Conserved current and probability

The concept of conserved current is simple and natural. When there is anything that 'exists' and 'moves around' in space and if it is not created or destroyed, then there is a conserved current. The electric charge and the classical density of gas flow are some examples. In particular we expect that the probability density of a wave fucntion to have such property. Thus, our strategy is to look for a conserved quantity for a given wave equation, and attempt to interpret it as the probability current.

Let's formulate the concept of conserved current more precisely. First, assume that there is some density of some 'material' $\rho(t, \vec{x})$ measured in a given frame which we call 'the laboratory frame' without loss of generaility. Then, one can form a 3-vector 'flux' defined by

$$\vec{j}(t, \vec{x}) \stackrel{\text{def}}{\equiv} \rho(t, \vec{x})\vec{\beta}(t, \vec{x}) \tag{2.5}$$

where $\beta(t, \vec{x})$ is the velocity of this 'material' at $(t, \vec{x})$. Then the quantity that flows across a small area $d\vec{a}$, which is fixed in the laboratory frame, is given by



$$\vec{j} \cdot d\vec{a} \qquad (\text{flow across } d\vec{a}) \tag{2.6}$$

No net creation nor destruction of the material means that, if we fix a volume V in space, the change in the total amount of the material in the volume, $\int_V \rho dv$, is entirely accounted for by how much is flowing in across the boundary surface A of the volume. Namely,

$$\frac{d}{dt}\int_V \rho(t, \vec{x})dv = -\int_A \vec{j} \cdot d\vec{a} \tag{2.7}$$

or moving the time derivative to the inside of the integral and using the Gauss's theorem (which is correct for any $\vec{j}$, conserved or not) on the right hand side,

$$\int_V \frac{d}{dt}\rho(t, \vec{x})dv = -\int_V \vec{\nabla} \cdot \vec{j} dv\,. \tag{2.8}$$

Since this should hold for any volume V, the integrands should be equal point by point:

$$\frac{d\rho}{dt} + \vec{\nabla} \cdot \vec{j} = 0\,. \tag{2.9}$$

Note that ρ could in general have negative values such as in the case of the electric charge.

If we define a 4-component quantity $j^\mu \equiv (\rho, \vec{j})$, then (2.9) above can be written as $\partial_\mu j^\mu = 0$, which looks like Lorentz-invariant. This, however, is true only if j^μ transforms as a Lorentz 4-vector, which is the case for the electric charge current as we have seen, or similarly for any flow of some realistic material such as gas flow.

2.3 The Schrödinger equation

Let's briefly review how the Schrödinger equation was introduced and how the probability density was defined. In the classical mechanics, the energy of a particle in the absence of interactions is given by

$$E = \frac{\vec{P}^2}{2m}\,. \tag{2.10}$$

The Schrödinger equation is then obtained by replacing E by $i\partial/\partial t$ and $\vec{P}$ by $-i\vec{\nabla}$ in the above and let them act on a complex scalar function $\phi(x)$ with $x^\mu = (t, \vec{x})$:

$$i\frac{\partial}{\partial t}\phi(x) = -\frac{1}{2m}\nabla^2\phi(x)\,. \quad \text{(Schrödinger equation)} \tag{2.11}$$

When applied to the plane-wave form (2.2), the operator $i\partial/\partial t$ 'pulls down' a factor E from the exponent, and the operator $-i\vec{\nabla}$ 'pulls down' a factor $\vec{P}$. Thus, if we substitute the plane-wave form in the above, we recover the relation between energy and momentum. The solution of the Schrödinger equation with given energy and momentum is then

$$\phi(x) = Ne^{-i(Et-\vec{P}\cdot\vec{x})}, \quad \text{with} \quad E = \frac{\vec{P}^2}{2m}, \tag{2.12}$$

where N is a normalization constant. Namely, the plane-wave form becomes a solution of the Schrödinger equation when the constants E and $\vec{P}$ in the exponent are related by $E = \vec{P}^2/2m$.

Next, a conserved quantity, which is interpreted as the probability density, can be constructed as follows: Multiplying ϕ^* to (2.11) from the left, we get

$$i\phi^*\Big(\frac{\partial}{\partial t}\phi\Big) = -\frac{1}{2m}\phi^*(\nabla^2\phi) \tag{2.13}$$

Taking the complex conjugate of (2.11) and multiplying ϕ from the right, we get

$$-i\Big(\frac{\partial}{\partial t}\phi^*\Big)\phi = -\frac{1}{2m}(\nabla^2\phi^*)\phi\,. \tag{2.14}$$

Subtracting (2.14) from (2.13),

$$\underbrace{i\Big[\phi^*\Big(\frac{\partial}{\partial t}\phi\Big)+\Big(\frac{\partial}{\partial t}\phi^*\Big)\phi\Big]}_{\frac{\partial}{\partial t}(\phi^*\phi)} = -\frac{1}{2m}\underbrace{\Big[\phi^*(\nabla^2\phi)-(\nabla^2\phi^*)\phi\Big]}_{\vec{\nabla}\cdot\big[\phi^*(\vec{\nabla}\phi)-(\vec{\nabla}\phi^*)\phi\big]}\,, \tag{2.15}$$

where we have used on the right hand side $\vec{\nabla}\cdot(\phi\vec{A}) = \vec{\nabla}\phi\cdot\vec{A}+\phi\vec{\nabla}\cdot\vec{A}$:

$$\begin{aligned}\vec{\nabla}\cdot\Big[\phi^*(\vec{\nabla}\phi)-(\vec{\nabla}\phi^*)\phi\Big] &= \phi^*(\nabla^2\phi)+\vec{\nabla}\phi^*\cdot\vec{\nabla}\phi-\vec{\nabla}\phi^*\cdot\vec{\nabla}\phi-(\nabla^2\phi^*)\phi \\ &= \phi^*(\nabla^2\phi)-(\nabla^2\phi^*)\phi\,. \end{aligned} \tag{2.16}$$

Then, (2.15) can be written as

$$\frac{\partial}{\partial t}\rho = -\vec{\nabla}\cdot\vec{j} \tag{2.17}$$

with

$$\rho = \phi^*\phi, \qquad \vec{j} = -\frac{i}{2m}\Big[\phi^*(\vec{\nabla}\phi)-(\vec{\nabla}\phi^*)\phi\Big]\,. \tag{2.18}$$

Thus, assuming that ϕ satisfies the Schrödinger equation, the quantities $(\rho,\vec{j})$ defined this way satisfy the same equation of conservation (2.9) introduced for a flow of some classical material. There, the density ρ and the current $\vec{j}$ were related by $\vec{j} = \rho\vec{\beta}$. What is $\vec{\beta}$ in the case of the Schrödinger equation? Using the plane-wave solution (2.12) in the definition of ρ and $\vec{j}$ above, we get

$$\rho = |N|^2, \quad \vec{j} = -\frac{i}{2m}|N|^2\Big[(i\vec{P})-(-i\vec{P})\Big] = |N^2|\frac{\vec{P}}{m}\,; \tag{2.19}$$

thus,

$$\vec{j} = \frac{\vec{P}}{m}\,\rho\,. \tag{2.20}$$

Since $\vec{\beta} = \vec{P}/m$ in classical mechanics, this indeed corresponds to $\vec{j} = \rho\vec{\beta}$. Note also that the density $\rho = |N|^2$ is always positive. Thus, the conserved current defined for the Schrödinger equation as (2.18) can be interpreted as the probability current.

The Schrödinger equation, however, is not Lorentz-invariant; namely, if we use the 4-vector nature of the operator ∂_μ and the scalar nature of the field ϕ [see (1.68) and the discussion that immediately follows it]:

$$\partial_\mu = \Lambda_\mu{}^\nu\partial_\nu, \quad \phi'(x') = \phi(x) \quad (x'^\mu = \Lambda^\mu{}_\nu x^\nu), \tag{2.21}$$

then, the Schrödinger equation in one frame does not lead to the same form of equation in the Lorentz-transformed frame:

$$i\frac{\partial}{\partial t}\phi(x) = -\frac{1}{2m}\nabla^2\phi(x) \quad \not\to \quad i\frac{\partial}{\partial t'}\phi'(x') = -\frac{1}{2m}\nabla'^2\phi'(x')\,; \tag{2.22}$$

where $\vec{\nabla}'$ denotes the derivatives with respect to the primed coordinates. Rather, it ends up in a terrible mess. Similarly, under the same transformation given by (2.21), the 4-component quantity $j^\mu = (\rho, \vec{j})$, where ρ and $\vec{j}$ are defined as (2.18), does not transform as a 4-vector:

$$j'^\mu(x') \neq \Lambda^\mu{}_\nu j^\nu(x), \tag{2.23}$$

which can easily be seen by noting that ρ as defined here is a scalar quantity: using $\phi'(x') = \phi(x)$,

$$\rho'(x') \equiv \phi'^*(x')\phi'(x') = \phi^*(x)\phi(x) = \rho(x)\,. \tag{2.24}$$

Thus, $j^0 = \rho$ cannot be the time component of a 4-vector which has to mix with space components under a general Lorentz transformation.

2.4 Klein-Gordon equation

In order to look for a Lorentz-invariant wave equation, we start from the relativistic energy-momentum relation for a particle

$$E^2 = \vec{P}^2 + m^2\,, \tag{2.25}$$

and apply the substitution (2.1) as in the case of the Schrödinger equation to get

$$-\frac{\partial^2}{\partial t^2}\phi(x) = (-\nabla^2 + m^2)\phi(x)\,, \tag{2.26}$$

or

$$\boxed{(\partial_\mu \partial^\mu + m^2)\phi(x) = 0\,,} \tag{2.27}$$

where

$$\partial_\mu \partial^\mu = \partial_0\partial^0 + \partial_1\partial^1 + \partial_2\partial^2 + \partial_3\partial^3 = \frac{\partial^2}{\partial t^2} - \nabla^2\,. \tag{2.28}$$

This equation (2.27) is called the Klein-Gordon equation. The operator $\partial_\mu\partial^\mu$ is sometimes written in different ways:

$$\partial_\mu\partial^\mu \equiv \partial^2 \equiv \Box \tag{2.29}$$

and called the D'Alembertian operator.

Now, the equation (2.27) looks Lorentz-invariant, and indeed it is. Using the transformation (2.21),

$$\begin{aligned} \partial'_\mu \partial'^\mu \phi'(x') &= (\Lambda_\mu{}^\alpha \partial_\alpha)(\Lambda^\mu{}_\beta \partial^\beta)\phi(x) \\ &= \underbrace{\Lambda_\mu{}^\alpha \Lambda^\mu{}_\beta}_{g^\alpha{}_\beta} \partial_\alpha \partial^\beta \phi(x) = \partial_\alpha \partial^\alpha \phi(x)\,. \end{aligned} \tag{2.30}$$

Thus, if a wave function $\phi(x)$ satisfy the Klein-Gordon equation in one frame, then the same form of equation is satified by the transformed wave function $\phi'(x')$ provided that $\phi(x)$ transforms as a scalar field [namely, $\phi'(x') = \phi(x)$]:

$$(\partial^2 + m^2)\phi(x) = 0 \quad \to \quad (\partial'^2 + m^2)\phi'(x') = 0\,. \tag{2.31}$$

Thus, the Klein-Gordon equation is Lorentz-invariant.

Next, let's examine the sign of the energy for solutions of the Klein-Gordon equation. To do so, we will again try the plane-wave form (2.2), this time expressed using the energy-momentum 4-vector:

$$\phi(x) = Ne^{-i(Et-\vec{P}\cdot\vec{x})} = Ne^{-ip\cdot x}, \qquad [p^\mu \equiv (E, \vec{P})] \tag{2.32}$$

Noting that

$$\partial_\mu(p\cdot x) = \frac{\partial}{\partial x^\mu}(p_\nu x^\nu) = p_\nu \underbrace{\frac{\partial x^\nu}{\partial x^\mu}}_{\delta_{\mu\nu}} = p_\mu\,, \tag{2.33}$$

$$\to \quad \partial_\mu e^{-ip\cdot x} = -ip_\mu e^{-ip\cdot x}\,, \tag{2.34}$$

we get

$$(\partial_\mu\partial^\mu + m^2)\phi = (\underbrace{(-ip_\mu)(-ip^\mu)}_{-p^2} + m^2)\phi = 0 \quad \to \quad p^2 = m^2\,, \tag{2.35}$$

which is nothing but the relativistic energy-momentum relation (2.25). Namely, a plane-wave (2.32) is a solution of the Klein-Gordon equation as long as the constants E and $\vec{P}$ satisfy the relation $E^2 = \vec{P}^2 + m^2$.

In contrast to the case of the Schrödinger equation where the condition $E = \vec{P}^2/2m$ required that E be positive, in this case E can be positive or negative. One way to get around the negative energies may be simply not to use the negative-energy solutions. However, when interactions are included in the theory, it turns out that the theory will *predict* that the positive energy states will eventually fall into the negative energy states (by emitting photons, for example).

Leaving the negative-energy problem as it is, let's turn to the conserved current of the Klein-Gordon theory in order to study the sign of the probability. Multiplying the Klein-Gordon equation (2.27) with ϕ^* on the left, and multiplying the complex conjugate of (2.27) with ϕ on the right, we get

$$\phi^*(\partial_\mu\partial^\mu\phi) + m^2\phi^*\phi \;=\; 0 \tag{2.36}$$

$$(\partial_\mu\partial^\mu\phi^*)\phi + m^2\phi^*\phi \;=\; 0\,. \tag{2.37}$$

Taking the difference of the two, we have

$$\begin{aligned} 0 &= \phi^*(\partial_\mu \partial^\mu \phi) - (\partial_\mu \partial^\mu \phi^*)\phi \\ &= \Big[\phi^*(\partial_\mu \partial^\mu \phi) + \partial_\mu \phi^* \partial^\mu \phi\Big] - \Big[\partial_\mu \phi^* \partial^\mu \phi + (\partial_\mu \partial^\mu \phi^*)\phi\Big] \\ &= \partial_\mu \Big[\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*)\phi\Big]\,. \end{aligned} \tag{2.38}$$

Thus, we have a conserved current

$$\partial_\mu j^\mu = 0\,, \tag{2.39}$$

where the current j^μ is defined by

$$j^\mu = i\,[\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*)\phi]\,, \tag{2.40}$$

which can be symbolically written as

$$\boxed{j^\mu = i\,\phi^* \overleftrightarrow{\partial}^\mu \phi}\,, \tag{2.41}$$

The symbol $\overleftrightarrow{\partial}^\mu$ used above is defined by

$$a\,\overleftrightarrow{\partial}^\mu b \stackrel{\text{def}}{\equiv} a(\partial^\mu b) - (\partial^\mu a)b\,; \tag{2.42}$$

namely, it operates on everything to the right and then everything to the left with a minus sign. Note that the second term in (2.40) is the complex conjugate of the first term. The factor 'i' in (2.40) is added to make j^μ a real quantity.

Using the plane-wave form (2.32) in (2.40),

$$j^\mu = i|N|^2[(-ip^\mu) - (ip^\mu)] = 2|N|^2 p^\mu\,. \tag{2.43}$$

The time component is then supposed to be the probability density:

$$j^0 = 2|N|^2 E \tag{2.44}$$

which can be both positive or negative since E can be positive or negative as discussed earlier.

Thus, in the Klein-Gordon theory, the problem of negative energy and that of negative probability are related. For the probability current, a natural question is whether one can construct a conserved current whose time component is always positive. People have tried, and were not successful. The true resolution of these problems will be accomplished in the framework of the quantum field theory. There, the probability current defined above will be reinterpreted as the charge current which can naturally be negative, and the energy becomes the eigenvalue of the Hamiltonian operator, which turns out to be always positive. Then, what happens to the probability density in the quantum field theory? In a nut shell, the concept of the probability that a particle is found at a given position loses its usefulness since particle and anti-particle can be pair-created out of vacuum for a short period of time, which is a result of the multi-particle nature of the quantum field theory as opposed to the single-particle nature of the quantum mechanical wave function which describes a state of a only one particle. For now, we will stay within the framework of the quantum mechanical wave function, and move on to the wave equation for a spin 1/2 particle - the Dirac equation.