The Free Klein Gordon Field Theory

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Abstract

A single-particle relativistic theory turns out to be inadequate for many situations. Thus, we begin to develop a multi-particle relativistic description of quantum mechanics starting from classical analogies. We start with a Lagrangian description, and use it to build a Hamiltonian description we can then quantize. We then illustrate the decomposition of the field into its positive and negative energy components, and define the creation and annihilation operators.

1 Introduction

Relativistic quantum mechanics turns out to be inadequately described by a single-particle theory. One of the primary reasons for this is that a relativistic particle may have enough energy to create other particles, and thus any theory describing it must account for this.

A theory which describes an infinite-degree-of-freedom system could be built out of a function defined over all space and time, similarly to the way such things are modeled in electromagnetic theory. From such a theory, we would need to find two major descriptions/properties: dynamical equations of motion and quantization. For the first, we can develop a Lagrangian description, and for the second, a Hamiltonian description lends itself quite well to quantization.

We will assume we have a field variable $\phi(x) = \phi(\mathbf{x}, t)$ which is real and behaves as a scalar under Lorentz transformation, and drops off to 0 at spatial infinity (as well as its derivatives).

2 Klein-Gordon from a Lagrangian

We first ask if there is a Lagrangian for the field $\phi(x)$ from which we can derive the Klein-Gordon equation by the principle of least action. We can actually solve this classically.

First, we assume there exists a Lagrangian density $\mathcal{L}$ defined as

$$L = \int d^3x \mathcal{L} \tag{1}$$

We will assume there exists an action S defined as normal, which we can write in terms of $\mathcal{L}$:

$$S = \int_{t_i}^{t_f} dt\, L = \int_{t_i}^{t_f} dt\, d^3x\, \mathcal{L} = \int_{t_i}^{t_f} d^4x\, \mathcal{L} \tag{2}$$

We will further assume that $\mathcal{L}$ depends only on the field variable and its first derivative, i.e.

$$\mathcal{L} = \mathcal{L}(\phi(x), \partial_\mu \phi(x)) \tag{3}$$

Now we will change the field arbitrarily and infinitesimally to find what conditions will result in a stationary action

$$\phi(x) \quad \rightarrow \quad \phi\prime(x) = \phi(x) + \delta\phi(x) \tag{4}$$

and apply the vanishing boundary condition

$$\delta\phi(\mathbf{x}, t_i) = \delta\phi(\mathbf{x}, t_f) = 0 \tag{5}$$

Now we can look at an infinitesimal change in S:

$$\delta S = \int_{t_i}^{t_f} d^4x\, \delta\mathcal{L} \tag{6}$$

We can expand this using the total derivative of $\mathcal{L}$:

$$= \int_{t_i}^{t_f} d^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \delta(\partial_\mu \phi(x)) \right) \tag{7}$$

If we commute δ and ∂_μ (it can be shown fairly easily that we can do this):

$$= \int_{t_i}^{t_f} d^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \partial_\mu(\delta\phi(x)) \right) \tag{8}$$

Then, we integrate the second term by parts $\left(\text{splitting up into } \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \text{ and } \partial_\mu(\delta\phi(x))\right)$ to obtain

$$= \int_{t_i}^{t_f} d^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \right) - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial \partial_\mu \phi(x)} \right) \delta\phi(x) \right) \tag{9a}$$

$$= \int_{t_i}^{t_f} d^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \right) \delta\phi(x) + \int d^3x\, \frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) \bigg|_{t_i}^{t_f} \tag{9b}$$

The second integral vanishes from the boundary conditions, so we're just left with the first term. To make the action stationary in the case of an arbitrary infinitesimal change in $\phi(x)$, it must be true that

$$\frac{\partial \mathcal{L}}{\partial \phi(x)} = \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \tag{10}$$

which is a generalization of the Euler-Lagrange equation for a field variable.

We will pick the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 \tag{11}$$

This choice can be motivated by looking at the Lagrangian for a classical harmonic oscillator,

$$L = \frac{1}{2}mv^2 - \frac{1}{2}m\omega^2x^2 \tag{12}$$

We see that if we treat $\phi(x)$ as x, $\partial_\mu\phi$ is analogous to v, and doing so gives us (11).

Evaluating both sides to be

$$\frac{\partial\mathcal{L}}{\partial\phi(x)} = -m^2\phi(x) \tag{13a}$$

$$\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi(x)} = \frac{\partial}{\partial\partial_\mu\phi}\left(\frac{1}{2}\partial_\mu\phi\eta^{\nu\mu}\partial_\nu\phi\right) \tag{13b}$$

$$= \frac{1}{2}\eta^{\nu\mu}\left(\left(\frac{\partial}{\partial\partial_\mu\phi}\partial_\mu\phi\right)\partial_\nu\phi + \partial_\mu\phi\left(\frac{\partial}{\partial\partial_\mu\phi}\partial_\nu\phi\right)\right) \tag{13c}$$

$$= \frac{1}{2}\eta^{\nu\mu}\left(\partial_\nu\phi + \partial_\mu\phi\delta^\mu_\nu\right) \tag{13d}$$

$$= \frac{1}{2}\eta^{\nu\mu}\left(2\partial_\nu\phi\right) \tag{13e}$$

$$= \partial^\mu\phi \tag{13f}$$

We find that (10) gives us

$$-m^2\phi = \partial_\mu\partial^\mu\phi \quad \rightarrow \quad (\partial_\mu\partial^\mu + m^2)\phi = 0 \tag{14}$$

Thus, the Klein-Gordon equation can be derived solely from the Lagrangian mechanics of our field operator ϕ.

3 Quantizing the Field

Now we want to actually quantize ϕ, similarly to how x and p are quantized in the simpler formulation of quantum theory. This is referred to as "second quantization". We can do this by creating a Hamiltonian description of ϕ in a similar way to how it is done classically, but treating q as ϕ and $\dot{q}$ as $\partial_\mu\phi$.

We will define the momentum operator as

$$\Pi(x) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} \tag{15}$$

and the Hamiltonian density as

$$\mathcal{H} = \Pi(x)\partial_\mu\phi(x) - \mathcal{L} \tag{16}$$

with the Hamiltonian itself defined as

$$H = \int d^3x \, \mathcal{H} \tag{17}$$

Clearly, these are defined very similarly to their classical definitions.

Now, as in classical mechanics, we will assume that the equal time Poisson bracket relations between ϕ and Π are

$$\{\phi(x), \phi(y)\}_{x^0=y^0} = 0 = \{\Pi(x), \Pi(y)\}_{x^0=y^0} \tag{18}$$
$$\{\phi(x), \Pi(y)\}_{x^0=y^0} = \delta^3(x-y) \tag{19}$$

This is again inspired by the classical case, which has that

$$\begin{aligned} \{x, x\} &= 0 = \{p, p\} \\ \{x, p\} &= 1 \end{aligned}$$

We can use these relations to write (after a semi-involved process) the Klein-Gordon equation in Hamiltonian form.

First, the Lagrangian density can give us the Hamiltonian density:

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 \tag{11 again}$$
$$= \frac{1}{2}\dot{\phi}^2 - \frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) - \frac{1}{2}m^2\phi^2 \tag{20}$$
$$\to \Pi(x) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \dot{\phi}(x) \tag{21}$$
$$\to \mathcal{H} = \Pi(x)\dot{\phi}(x) - \mathcal{L} \tag{16 again}$$
$$= \Pi^2(x) - \left(\frac{1}{2}\Pi^2(x) - \frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) - \frac{1}{2}m^2\phi^2\right) \tag{22}$$
$$= \frac{1}{2}\Pi^2(x) + \frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) + \frac{1}{2}m^2\phi^2 \tag{23}$$

This in turn gives us the Hamiltonian

$$H = \int d^3x \, \mathcal{H} \tag{17 again}$$
$$= \int d^3x \left(\frac{1}{2}\Pi^2(x) + \frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) + \frac{1}{2}m^2\phi^2\right) \tag{24}$$

Now again, analogously to the classical case, we will look at Hamilton's equations with ϕ:

$$\begin{aligned}
\dot{\phi}(x) &= \{\phi(x), H\} \\
&= \left\{\phi(x), \int d^3y \left(\frac{1}{2}\Pi^2(y) + \frac{1}{2}(\nabla\phi(y))\cdot(\nabla\phi(y)) + \frac{1}{2}m^2\phi^2\right)\right\} \\
&= \frac{1}{2}\int d^3x \, \{\phi(x), \Pi^2(y)\}_{x^0=y^0} \\
&= \int d^3y \, \Pi(y)\{\phi(x), \Pi^2(y)\}_{x^0=y^0} \\
&= \int d^3y \, \Pi(\mathbf{y}, x^0)\{\phi(x), \Pi(y)\}_{x^0=y^0} \\
&= \int d^3y \, \Pi(\mathbf{y}, x^0)\delta^3(x-y) \\
&= \Pi(x)
\end{aligned} \tag{25}$$

Here we have used that the Hamiltonian is time-independent, so we can assert that $x^0 = y^0$, allowing us to use the equal-time relation (19). We can go through a similar process to find $\dot{\Pi}$:

$$\begin{aligned}
\dot{\Pi}(x) &= \{\Pi(x), H\} \\
&= \left\{\Pi(x), \int d^3y \left(\frac{1}{2}\Pi^2(y) + \frac{1}{2}(\nabla\phi(y))\cdot(\nabla\phi(y)) + \frac{1}{2}m^2\phi^2\right)\right\} \\
&= \int d^3y \, (\nabla\phi(y)\cdot\{\Pi(x), \nabla\phi(y)\}_{x^0=y^0} \\
&\qquad\qquad + m^2\phi(y)\{\Pi(x), \phi^2(y)\}_{x^0=y^0}) \\
&= \int d^3y \, (\nabla\phi(\mathbf{y}, x^0)\cdot\nabla(-\delta^3(x-y)) \\
&\qquad\qquad + m^2\phi(\mathbf{y}, x^0)(-\delta^3(x-y))) \\
&= \nabla\cdot\nabla\phi(x) - m^2\phi(x) = \nabla^2\phi(x) - m^2\phi(x)
\end{aligned} \tag{26}$$

These first-order Hamilton equations give us the second-order equation

$$\begin{aligned}
\ddot{\phi}(x) &= \dot{\Pi}(x) = \nabla^2\phi(x) - m^2\phi(x) \\
&\rightarrow (\ddot{\phi} - \nabla^2\phi(x)) + m^2\phi(x) = 0 \\
&\rightarrow (\partial_\mu\partial^\mu + m^2)\phi(x) = 0
\end{aligned} \tag{27}$$

Thus, this Hamiltonian description *also* brings about the Klein-Gordon equation.

Finally, we can quantize by treating ϕ and Π as Hermitian operators satisfying the following equal-time commutation relations:

$$[\phi(x), \phi(y)]_{x^0=y^0} = 0 = [\Pi(x), \Pi(y)]_{x^0=y^0} \tag{28}$$

$$[\phi(x), \Pi(y)]_{x^0,y^0} = i\delta^3(x-y) \tag{29}$$

This is the second-quantization we were looking for.

4 Field Decomposition

The following plane wave equation set forms a complete basis for solutions to the Klein-Gordon equation [1]:

$$\phi(x) = e^{-ik\cdot x} \tag{30}$$

We can use this basis to expand ϕ in this basis:

$$\phi(x) = C\int d^4k\, e^{-ik\cdot x}\tilde{\phi}(k) \quad ; \quad C = \frac{1}{(2\pi)^{\frac{3}{2}}} \tag{31}$$

This is essentially a Fourier transform of $\tilde{\phi}(k)$, with C introduced for later convenience. We can now plug this into the Klein-Gordon equation:

$$\begin{aligned}
&C(\partial_\mu\partial^\mu + m^2)\int d^4k\, e^{-ik\cdot x}\tilde{\phi}(k) = 0 \\
&\to C\int d^4k\, (\partial_\mu\partial^\mu + m^2)e^{-ik\cdot x}\tilde{\phi}(k) = 0 \\
&\to C\int d^4k\, (-k^2 + m^2)\tilde{\phi}(k)e^{-ik\cdot x} = 0
\end{aligned} \tag{32}$$

So at least one of the following must be true:

$$k^2 = m^2 \tag{33}$$

$$\tilde{\phi}(k) = 0 \tag{34}$$

So, $\tilde{\phi}$ is only non-vanishing when $k^2 = m^2$; we'll define $\tilde{\phi}$ in the following way to capture this:

$$\tilde{\phi}(k) = \delta(k^2 - m^2)a(k) \tag{35a}$$

$$\to \phi(x) = C\int d^4k\, \delta(k^2 - m^2)e^{-ik\cdot x}a(k) \tag{35b}$$

Since this vanishes for

$$k^2 = m^2 \tag{36a}$$

$$\to (k^0)^2 = \mathbf{k} + m^2 \tag{36b}$$

$$\to k^0 = \pm\sqrt{\mathbf{k}^2 + m^2} = \pm E_k, \tag{36c}$$

we can rewrite the delta function using the property that

$$\delta(g(x)) = \sum_i \frac{\delta(x - x_i)}{|g\prime(x_i)|} \tag{37}$$

$$\begin{aligned}
\to \delta(k^2 - m^2) &= \delta((k^0)^2 - E_k^2) \\
&= \frac{1}{2|k^0|}(\delta(k^0 - E_k) + \delta(k^0 + E_k)) \\
&= \frac{1}{2E_k}(\delta(k^0 - E_k) + \delta(k^0 + E_k))
\end{aligned} \tag{38}$$

Now we can plug this new form into (35b):

$$\begin{aligned}\phi(x) = C \int dk^0\, d^3k\, \frac{1}{2E_k}(\delta(k^0 - E_k) + \delta(k^0 + E_k)) \\ \times e^{-i(k^0x^0 - \mathbf{k}\cdot\mathbf{x})} a(k^0, \mathbf{k}) \\ = C \int d^3k\, \frac{1}{2E_k} \left(e^{i(-E_k x^0 + \mathbf{k}\cdot\mathbf{x})} a(E_k, \mathbf{k}) + e^{i(E_k x^0 + \mathbf{k}\cdot\mathbf{x})} a(-E_k, \mathbf{k})\right) \end{aligned} \tag{39}$$

We will replace E_k with k^0 and switch $\mathbf{k}$ to $-\mathbf{k}$ in the second term to obtain

$$\phi(x) = C \int d^3k\, \frac{1}{2E_k} \left(e^{-ik\cdot x} a(k) + e^{ik\cdot x} a(-k)\right) \tag{40}$$

Since ϕ is Hermitian,

$$\begin{aligned}\phi(x) &= \phi^\dagger(x) \\ &= C \int d^3k\, \frac{1}{2E_k} \left(e^{ik\cdot x} a^\dagger(k) + e^{-ik\cdot x} a^{dagger}(-k)\right)\end{aligned} \tag{41}$$

Combining (40) with (41), we get that

$$a(k) = a^\dagger(-k) \quad \text{and} \quad a(-k) = a^\dagger(k) \tag{42}$$

Now we can rewrite (40) as

$$\phi(x) = C \int d^3k\, \frac{1}{2E_k} \left(e^{-ik\cdot x} a(k) + e^{ik\cdot x} a^\dagger(k)\right) \tag{43}$$

From (36c), we know that $k^0 = k^0(\mathbf{k})$, so we can redefine $a(k)$ to reflect this:

$$a(\mathbf{k}) = \frac{a(k)}{\sqrt{2k^0}} \quad \text{and} \quad a^\dagger(\mathbf{k}) = \frac{a^\dagger(k)}{\sqrt{2k^0}} \tag{44}$$

Using these new definitions, we will rewrite $phi(x)$ once more as

$$\phi(x) = D \int d^3k\, \left(e^{-ik\cdot x} a(\mathbf{k}) + e^{ik\cdot x} a^\dagger(\mathbf{k})\right) \quad ; \quad D = \frac{1}{\sqrt{(2\pi)^3 2k^0}} \tag{45}$$

We can denote $\phi(x)$ in terms of its positive and negative energy parts:

$$\phi^{(+)}(x) = D \int d^3k\, \left(e^{-ik\cdot x} a(\mathbf{k})\right) \tag{46a}$$

$$\phi^{(-)}(x) = D \int d^3k\, \left(e^{ik\cdot x} a^\dagger(\mathbf{k})\right) \tag{46b}$$

$$\to \phi(x) = \phi^{(+)}(x) + \phi^{(-)}(x) \tag{46c}$$

This is called the *decomposition* of ϕ, and it allows us to look at its positive and negative energy components on their own.

We also defined $a(k)$ and $a^\dagger(k)$ during this process. These are the annihilation and creation operators, which are analogous to the ladder operators for harmonic oscillators. They become very important to analyzing the behavior of the field. For more information, see Saltzman (2018) [2].

References

[1] Ashok Das. *Lectures on Quantum Field Theory.* World Scientific, 2008.

[2] Ben Saltzman. Second quantization of the klein-gordon equation. 2018.