Klein Gordon Field as Harmonic Oscillators and the Problem of Causality in 4 Dimensional Spacetime

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Term Paper
Quantum Mechanics

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Abstract

In this term paper, we try to understand the Klein Gordon Field Theory, illuminating its representation as a harmonic oscillator and understand its quantization which leads to the formation of Particles and Anti-Particles.Then we dive into the intricate problem of Causality within the realm of four dimensional spacetime.

Contents

1 Introduction

Quantum Field Theory is the quantization of the classical field just like quantum mechanics which is concerned mainly with the quantization of dynamical systems of particle. Quantization of fields helps in understanding processes that occur at quantum scales and very large energies (relativistic).

Although it should be noted that we cannot quantize relativistic particles in the same way we quantize non-relativistic particles. The reason is, the combination of Quantum Mechanics and Special Relativity implies that the particle number is not conserved. In other words, no relativistic processes can be explained in terms of single particle.

The Einstein relation $E = mc^2$ allows for the creation of particle and anti-particle pairs. This happens because energy is converted into mass. This energy is used to create rest mass of new particles. Furthermore, for every particle created, an antiparticle is also formed to conserve certain fundamental quantities such as electric charge, lepton number etc. They exist for a very short duration due to Energy-time uncertainty relation $\Delta E \Delta t \sim h$.

There is no mechanism in standard non-relativistic Quantum Mechanics to deal with changes in particle number. Constructing Schrodinger equation for single relativistic particle will have several problems like negative probabilities, infinite towers of negative energy states and breakdown in causality. For relativistic regime, we need a new formalism. This new formalism is Quantum Field Theory. One of the simplest type of classical field (which we will quantize) is what is known as the Klein Gordon field. We will see that the quantization of scalar fields gives rise to Bosons (spin 0 particles).

2 Lagrangian Field Theory

In field theory, Lagrangian is defined as,

$$\mathbf{L} = \int d^3x L(\phi, \partial_\mu \phi)$$

where L is the Lagrangian density. Although we will call it Lagrangian. The action can be written as

$$S = \int dt \mathbf{L} = \int dt \int d^3x L(\phi, \partial_\mu \phi)$$

$$S = \int d^4x L(\phi, \partial_\mu \phi)$$

The principle of Least Action tells that when system evolves from one configuration to other, it does so along a path in configurational space for which S is an extremum.

$$\delta S = 0$$

$$\int d^4x \left[\frac{\partial L}{\partial \phi} \delta\phi + \frac{\partial L}{\partial(\partial_\mu \phi)} \delta(\partial_\mu \phi) \right] = 0$$

$$\int d^4x \left[\frac{\partial L}{\partial \phi} - \partial_\mu \left(\frac{\partial L}{\partial(\partial_\mu \phi)} \right) \right] \delta\phi + \int d^4x \partial_\mu \left(\frac{\partial L}{\partial(\partial_\mu \phi)} \delta\phi \right) = 0$$

The second term will be 0 since $\delta\phi$ vanishes at the beginning and end of given field configuration. Since the integral is 0 for arbitrary $\delta\phi$, the quantity inside bracket must be 0 and we get the Euler Lagrangian Equation for the field.

$$\frac{\partial L}{\partial \phi} - \partial_\mu \left(\frac{\partial L}{\partial(\partial_\mu \phi)} \right) = 0$$

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Consider the following Lagrangian for the scalar field:

$$L = \frac{\dot{\phi}^2}{2} - \frac{(\nabla\phi)^2}{2} - \frac{m^2\phi^2}{2}$$

$$L = \frac{(\partial_\mu \phi)^2}{2} - \frac{m^2\phi^2}{2}$$

After applying Euler Lagrangian Equation, we get:

$$\left(\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2) \right) \phi = 0$$

$$OR$$

$$\left(\partial_\mu \partial^\mu + m^2 \right) \phi = 0$$

This is known as the Klein Gordon Equation.

3 Hamiltonian Field Theory

We define,

$$\pi(x) = \frac{\partial L}{\partial \dot{\phi}(x)}$$

where $\pi(x)$ is called momentum density conjugate to $\phi(x)$. Thus Hamiltonian is written as

$$\mathbf{H} = \int d^3 x H$$

$$\mathbf{H} = \int d^3 x \Big[\pi(x)\dot{\phi}(x) - L \Big]$$

For the Lagrangian given in previous section, canonical momentum conjugate to $\phi(x)$ is,

$$\pi(x) = \frac{\partial L}{\partial \dot{\phi}(x)} = \dot{\phi}(x)$$

Thus, Hamiltonian can be written as

$$\mathbf{H} = \int d^3 x \Big[\frac{\pi^2}{2} + \frac{(\nabla\phi)^2}{2} + \frac{m^2\phi^2}{2} \Big]$$

4 Canonical Quantization

It is the procedure to convert generalized co-ordinates of the system into operators. In field theory, we do this for the field $\phi_a(x)$ and $\pi_b(x)$. They are operator valued function of space obeying commutation relations.

$$\big[\phi_a(x), \pi^{\mathrm{b}}(y)\big] = i\delta^3(x-y)\delta_a{}^{\mathrm{b}}$$

$$\big[\phi_a(x), \phi_b(y)\big] = \big[\pi^{\mathrm{a}}(x), \pi^{\mathrm{b}}(y)\big] = 0$$

Note that we are now working in the Schrodinger picture. So operators ϕ and π do not depend on time but only space. Although $\mid \psi >$ depends on time and they evolve by usual Schrodinger equation,

$$i\frac{d \mid \psi >}{dt} = H \mid \psi >$$

In quantum field theory, $\mid \psi >$ is a functional of every possible configuration of field ϕ.

4.1 Free Field Theory

One of the main information we want to know about quantum theory is the spectrum of Hamiltonian.It means all possible energy eigenvalues that the system can obtained and the corresponding eigenstates.In field theory, this is very hard, because the field has infinite number of degrees of freedom - at least one for every point in space.

Free Field theories refers to those particular fields where each degree of freedom evolves independently from all others. Now we will solve the Klein Gordon equation using this concept.

Klein Gordon Equation is given by:

$$\left(\partial_\mu \partial^\mu + m^2\right)\phi = 0$$

We take Fourier Transform of $\phi(x)$ to represent this as linear superposition of $\phi(p)$ (where p is momentum) such that each degree of freedom (p) decouple from each other.

$$\phi(\vec{x}, t) = \int \frac{d^3p}{(2\pi)^3} \phi(\vec{p}, t) e^{i\vec{p}.\vec{x}}$$

Substituting $\phi(\vec{x}, t)$ in Klein Gordon equation and on solving, we get the following equation:

$$\left[\frac{\partial^2}{\partial t^2} + (p^2 + m^2)\right]\phi(\vec{p}, t) = 0$$

We find that the above equation is the equation of simple harmonic oscillation with frequency $\omega_p = \sqrt{p^2 + m^2}$. We conclude that the general solution to the Klein Gordon Equation is the linear superposition of infinite number of simple harmonic oscillators, each vibrating at different frequency and amplitudes.

4.2 Free Scalar Field

To quantize $\phi(\vec{x}, t)$, we have to quantize infinite number of harmonic oscillators. We define two operators $a_{\vec{p}}$ and $a^\dagger_{\vec{p}}$ called annihilation and creation operators respectively for each Fourier mode of field.We write ϕ and π as linear sum of infinite numbers of $a_{\vec{p}}$ and $a^\dagger_{\vec{p}}$ such that the above commutation relations are satisfied.

$$\hat{\phi}(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \left(a_{\vec{p}} e^{i\vec{p}.\vec{x}} + a^\dagger_{\vec{p}} e^{-i\vec{p}.\vec{x}}\right)$$

$$\hat{\pi}(x) = \int \frac{d^3p}{(2\pi)^3} (-i) \sqrt{\frac{\omega_p}{2}} \left(a_{\vec{p}} e^{i\vec{p}.\vec{x}} - a^\dagger_{\vec{p}} e^{-i\vec{p}.\vec{x}}\right)$$

We find that to obtain the commutation relation for ϕ and π, the following commutation relations for $a_{\vec{p}}$ and $a^\dagger_{\vec{p}}$ has to be satisfied.

$$\left[a_{\vec{p}}, a^\dagger_{\vec{q}}\right] = (2\pi)^3 \delta^3(p - q)$$

$$\left[a_{\vec{p}}, a_{\vec{q}}\right] = \left[a^\dagger_{\vec{p}}, a^\dagger_{\vec{q}}\right] = 0$$

We can now obtain Hamiltonian in terms of $a_{\vec{p}}$ and $a^\dagger_{\vec{p}}$. After performing all the complicated calculations, we finally get the following:

$$H = \int \frac{d^3p}{(2\pi)^3}\omega_p \left[a^\dagger_{\vec{p}}a_{\vec{p}} + \frac{(2\pi)^3}{2}\delta^3(0)\right]$$

It seems like this Hamiltonian has a lot to say. Let's analyze it.

4.3 Vacuum

We define vacuum $\mid 0>$ by the fact that it is annihilated by all annihilated operators.

$$a_{\vec{p}} \mid 0 >= 0 \qquad \forall \ \vec{p}$$

Applying Hamiltonian operator on vacuum, we get the following:

$$\begin{aligned} H \mid 0 >&= E_0 \mid 0 > \\ &= \left[\int d^3p \frac{\omega_p}{2}\delta^3(0)\right] \mid 0 > \\ &= \infty \mid 0 > \end{aligned}$$

There are two different ∞'s present in the expression. The first arises due to the presence of $\delta^3(0)$ which is due to the fact that space is infinitely large. Infinity of this type is known as infrared divergence. We consider our theory in finite dimensional box of length L and takes the limit $L \to \infty$.

$$\begin{aligned} \delta^3(p=0) = \delta^3(0) &= \lim_{L\to\infty}\int_{-L/2}^{L/2}\frac{d^3x}{(2\pi)^3}e^{i\vec{p}.\vec{x}}\Big|_{\vec{p}=0} \\ &= \lim_{L\to\infty}\int_{-L/2}^{L/2}\frac{d^3x}{(2\pi)^3} \\ (2\pi)^3\delta^3(0) &= V \end{aligned}$$

This infinity is arising because we are calculating total energy rather than the energy density. Hence,

$$\frac{E_0}{V} = \epsilon_0 = \int \frac{d^3p}{(2\pi)^3}\frac{\omega_p}{2}$$

which is still infinite.If we observe carefully, we realize that ϵ_0 is the sum of infinite number of ground state energies. $\epsilon_0 \to \infty$ due to the fact that $p \to \infty$. This is a high frequency or short distance ∞ which is known as ultraviolet divergence.

To deal with both ∞'s, we simply remove (or shift) that term since we really concerned about energy differences from vacuum energy rather than the absolute energy. So we redefine Hamiltonian by,

$$H = \int \frac{d^3p}{(2\pi)^3} \omega_p a^\dagger_{\vec{p}} a_{\vec{p}}$$

such that $H \mid 0 >= 0$.

4.4 Particle and Multi-particle States

We now focus on the excitation of field. We know that,

$$[H, a_{\vec{p}}] = -\omega_{\vec{p}} a_{\vec{p}}$$

$$[H, a^\dagger_{\vec{p}}] = \omega_{\vec{p}} a^\dagger_{\vec{p}}$$

We can construct energy eigenstate by acting on vacuum $\mid 0 >$ with $a^\dagger_{\vec{p}}$.

$$\mid \vec{p} >= a^\dagger_{\vec{p}} \mid 0 >$$

This state has energy,

$$H \mid \vec{p} >= \omega_{\vec{p}} \mid \vec{p} >$$

where $\omega_{\vec{p}} = \sqrt{p^2 + m^2}$ which is nothing but the relativistic energy of particles (we are working in natural units, so c = h = 1).

$\mid p >$ here is the momentum eigenstate of single particle of mass m and momentum p. We can verify momentum by acting momentum operator $\hat{P}$ (we can obtain this with the help of Noether's Theorem).

$$\hat{P} = \int \frac{d^3p}{(2\pi)^3} \vec{p} a^\dagger_{\vec{p}} a_{\vec{p}}$$

$$\hat{P} \mid \vec{p} >= p \mid \vec{p} >$$

We can also know about the angular momentum of particle by acting angular momentum operator $\hat{J}$ (obtained from Noether's theorem) on $\mid \vec{p} >$ with 0 momentum. We obtain the following.

$$\hat{J} \mid \vec{p} = 0 >= 0$$

It shows that particle has no internal angular momentum. In other words, quantizing scalar field gives rise to spin 0 particles.

We can also create multi-particle state by acting multiple times with $a^\dagger_{\vec{p}}$ on vacuum.

$$\mid \vec{P}_1, ..., \vec{P}_n >= a^\dagger_{\vec{p_1}} ....a^\dagger_{\vec{p_n}} \mid 0 >$$

We get n particles state when n $a^\dagger_{\vec{p}}$'s act on vacuum. Since all $a^\dagger_{\vec{p}}$'s commute among themselves, the state will be symmetric under exchange of any 2 particles. For example, the two particle state $\mid \vec{p}, \vec{q} >$ and $\mid \vec{q}, \vec{p} >$ are identical since $a^\dagger_{\vec{p}}$ and $a^\dagger_{\vec{q}}$ commute among themselves. So order doesn't matter. Such particles are known as Bosons.

There is an operator called $\hat{N}$ which counts the number of particles in a given state.

$$\hat{N} = \int \frac{d^3p}{(2\pi)^3} a^\dagger_{\vec{p}} a_{\vec{p}}$$

$$\hat{N} \mid \vec{P}_1, ..., \vec{P}_n >= n \mid \vec{P}_1, ..., \vec{P}_n >$$

Also we find that [N,H] = 0 which ensures that the particle number is conserved. This is only true for free fields. Particle number is conserved here because the fields are not interacting with each other. Once interaction is introduced then particle numbers are no more conserved.

We conclude that the operator $a^\dagger_{\vec{p}}$ creates particles with momentum p and energy $\omega_p = \sqrt{p^2 + m^2}$. Similarly, the state $a^\dagger_{\vec{p}} a^\dagger_{\vec{q}} .... \mid 0 >$ has momentum p + q + ... We call these excitation particles, since they are discrete entities that have the proper relativistic energy-momentum relation.

Let us also interpret the state $\phi(x) \mid 0 >$. We know that,

$$\hat{\phi}(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \left(a_{\vec{p}} e^{i\vec{p}.\vec{x}} + a^\dagger_{\vec{p}} e^{-i\vec{p}.\vec{x}} \right)$$

$$\hat{\phi}(x) \mid 0 >= \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} e^{-i\vec{p}.\vec{x}} \mid p >$$

We interpret this expression as the linear superposition of infinite number of single particle states that have well defined momentum. This looks same as the familiar non-relativistic expression for the eigenstate of position $\mid x >$. We therefore conclude that the operator $\hat{\phi}(x)$,acting on the vacuum, creates a particle at position x.

So far we considered only real scalar fields. When we consider complex scalar fields, their quantization creates two types of particles, both of mass M and spin 0. They are particles and anti-particles. For real scalar fields, particle is its own anti-particle.

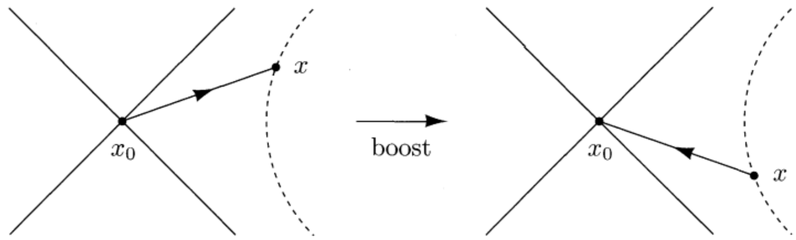

Figure 1: Propagation from x_0 to x in one frame looks like propagation from x to x_0 in another frame.

5 The Problem of Causality

Consider the amplitude for free particle to propagate from x_0 to x.

$$U(t) =< x \mid e^{-iHt} \mid x_0 >$$

For $E = \frac{p^2}{2m}$ (in non-relativistic regime),

$$\begin{aligned} U(t) &= \int \frac{d^3p}{(2\pi)^3} < x \mid e^{-i(\frac{p^2}{2m})t} \mid p >< p \mid x_0 > \\ &= \int \frac{d^3p}{(2\pi)^3} e^{-i(\frac{p^2}{2m})t} e^{ip(x-x_0)} \\ &= \left(\frac{m}{2\pi i t}\right)^{3/2} e^{im\frac{(x-x_0)^2}{2t}} \end{aligned}$$

$U(t) \neq 0 \quad \forall x, t$, which indicates that particle can propagate between any two points. But if we consider the energy in relativistic regime, i.e. $E = \sqrt{p^2 + m^2}$, this would violates the principle of Causality.

The principle of Causality asserts that no influence can travel faster than the speed of light. In other words, events occurring at one point in space-time, cannot instantly affects events occurring at another point that is spacelike separated that means events that are outside each other's light cones.

For $E = \sqrt{p^2 + m^2}$ (in relativistic regime),

$$\begin{aligned} U(t) &=< x \mid e^{-it(\sqrt{p^2+m^2})} \mid x_0 > \\ &= \int \frac{d^3p}{(2\pi)^3} e^{-it(\sqrt{p^2+m^2})} e^{ip(x-x_0)} \\ &\approx e^{-m\sqrt{x^2-t^2}} \end{aligned}$$

This integral can be evaluated with the help of Bessel's function. Here we find that the propagation amplitude is small but non-zero outside the light-cone and the principle of causality is violated.

Quantum Field Theory solves this problem.We find in multi-particle field theory that the propagation of particle across space-like interval is indistinguishable from the propagation of anti-particle in opposite direction. The amplitudes for particle and anti-particle propagation exactly cancel out, so Causality is preserved.

6 References

1) https://www.damtp.cam.ac.uk/user/tong/qft.html
2) An Introduction to Quantum Field Theory by Michael E. Peskin