Kapitza
Spring 2018

Second Quantization of the Klein-Gordon Equation

Ben Saltzman

Q.F.T. TERM PAPER

Professor Sarada Rajeev
April 20th 2017

1 Introduction

The Schrödinger equation, successful as it is for describing non-relativistic quantum particles, fails in the relativistic regime. By using special relativity, one can derive a relativistic version of the Schrödinger equation, known as the first quantization of the Klein-Gordon equation. Unfortunately, this has its own problems: negative energy and probability solutions, nonphysical entities that could spell the end for a theory. Moving from quantum theory to quantum field theory, fields are introduced as fundamental. Quantizing the Klein-Gordon equation in quantum field theory leads to a model known as the second quantization, which avoids many of the problems of the first quantization.

2 Second Quantization of the Klein-Gordon Equation

2.1 The Klein-Gordon Field

We can write the Klein-Gordon field operator as

$$\phi(\mathbf{x}) = C \int \mathrm{d}^3k \ \left(e^{(-i\mathbf{k}\cdot\mathbf{x})} a(\mathbf{k}) + e^{(i\mathbf{k}\cdot\mathbf{x})} a^\dagger(\mathbf{k}) \right) \tag{1}$$

where

$$C = \frac{1}{\sqrt{2k^0(2\pi)^3}} \tag{2}$$

and $k^0 = E_k$. The field operator satisfies the Klein-Gordon equation, i.e.

$$(\partial_\mu \partial^\mu + m^2)\phi = 0 \tag{3}$$

This can be split into positive and negative energy components as follows:

$$\begin{aligned} \phi(\mathbf{x}) &= \phi^{(+)}(\mathbf{x}) + \phi^{(-)}(\mathbf{x}) \\ \phi^{(+)}(\mathbf{x}) &= C \int \mathrm{d}^3k \ e^{(-i\mathbf{k}\cdot\mathbf{x})} a(\mathbf{k}) \\ \phi^{(-)}(\mathbf{x}) &= C \int \mathrm{d}^3k \ e^{(i\mathbf{k}\cdot\mathbf{x})} a^\dagger(\mathbf{k}) \end{aligned} \tag{4}$$

The conjugate momentum for the field operator is therefore

$$\begin{aligned} \Pi(\mathbf{x}) &= \dot{\phi}(\mathbf{x}) \\ &= -ik^0 C \int \mathrm{d}^3k \ \left(\exp(-i\mathbf{k}\cdot\mathbf{x}) a(\mathbf{k}) - \exp(i\mathbf{k}\cdot\mathbf{x}) a^\dagger(\mathbf{k}) \right) \end{aligned} \tag{5}$$

Inverting equations 1 and 5 and solving for the annihilation and creation operators a and $a^\dagger$:

$$\begin{aligned} a(\mathbf{k}) &= C \int \mathrm{d}^3x \;\; e^{i\mathbf{k}\cdot\mathbf{x}} \Big(k^0 \phi(\mathbf{x}) + i\Pi(\mathbf{x}) \Big) \\ &= iC \int \mathrm{d}^3x \;\; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \end{aligned} \tag{6}$$

$$\begin{aligned} a^\dagger(\mathbf{k}) &= C \int \mathrm{d}^3x \;\; e^{-i\mathbf{k}\cdot\mathbf{x}} \Big(k^0 \phi(\mathbf{x}) - i\Pi(\mathbf{x}) \Big) \\ &= -iC \int \mathrm{d}^3x \;\; \Big(e^{-i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{-i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \end{aligned} \tag{7}$$

Taking the time derivative of equation 6:

$$\begin{aligned} \partial_t a(\mathbf{k}) &= iC\partial_t \int \mathrm{d}^3x \;\; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \\ &= iC \int \mathrm{d}^3x \;\; \Big(\partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) + e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t^2 \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \\ &= iC \int \mathrm{d}^3x \;\; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t^2 \phi(\mathbf{x}) - \partial_t^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \end{aligned}$$

ϕ must satisfy the Klein-Gordon equation, so

$$\begin{aligned} \partial_t a(\mathbf{k}) &= iC \int \mathrm{d}^3x \;\; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} (\nabla^2 - m^2) \phi(\mathbf{x}) + (k^0)^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \\ &= iC \int \mathrm{d}^3x \;\; \Big((k^0)^2 - k^2 - m^2 \Big) e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \\ &= 0 \end{aligned}$$

since $(k^0)^2 - k^2 = m^2$. The same procedure follows for $a^\dagger$, meaning that the annihilation and creation operators are time independent.

The commutation relations between the annihilation and creation operators can be deduced from the already-known relations between the field operator and the conjugate momentum when imposing the contraint $x^0 = y^0$. To reduce clutter, we define $C' \equiv C\Big|_{k^0 \to k'^0}$.

$$
\begin{aligned}
[\phi(\mathbf{x}), \phi(\mathbf{y})] = CC' \iint \mathrm{d}^3k \ \ \mathrm{d}^3k' \ \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}), a(\mathbf{k}')] \\
& + e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}), a^\dagger(\mathbf{k}')\big] + e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a(\mathbf{k}')\big] \\
& + e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\big]\Big) \\
= 0 &
\end{aligned} \tag{8}
$$

$$
\begin{aligned}
[\Pi(\mathbf{x}), \Pi(\mathbf{y})] = -k^0 k'^0 CC' \iint \mathrm{d}^3k \ \ \mathrm{d}^3k' \ \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}), a(\mathbf{k}')] \\
& - e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}), a^\dagger(\mathbf{k}')\big] - e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a(\mathbf{k}')\big] \\
& + e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\big]\Big) \\
= 0 &
\end{aligned} \tag{9}
$$

$$
\begin{aligned}
[\phi(\mathbf{x}), \Pi(\mathbf{y})] = -ik'^0 CC' \iint \mathrm{d}^3k \ \ \mathrm{d}^3k' \ \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}), a(\mathbf{k}')] \\
& - e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}), a^\dagger(\mathbf{k}')\big] + e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a(\mathbf{k}')\big] \\
& - e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\big]\Big) \\
= i\delta^3(\mathbf{x}-\mathbf{y}) &
\end{aligned} \tag{10}
$$

The commutation relations between the annihilation and creation operators can be calculated from equations 6 and 7, knowing equations 2.1, 2.1, and 10:

$$
\begin{aligned}
[a(\mathbf{k}), a(\mathbf{k}')] = CC' \iint \mathrm{d}^3x \ \ \mathrm{d}^3y e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\Big(& k^0 k'^0[\phi(\mathbf{x}), \phi(\mathbf{y})] \\
& + ik^0[\phi(\mathbf{x}), \Pi(\mathbf{y})] + ik'^0[\Pi(\mathbf{x}), \phi(\mathbf{y})] - [\Pi(\mathbf{x}), \Pi(\mathbf{y})]\Big) \\
= CC' \iint \mathrm{d}^3x \ \ \mathrm{d}^3y e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})} & \Big(ik^0[\phi(\mathbf{x}), \Pi(\mathbf{y})] + ik'^0[\Pi(\mathbf{x}), \phi(\mathbf{y})]\Big) \\
= -CC'(k^0 - k'^0) \iint \mathrm{d}^3x \ \ \mathrm{d}^3y & e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\delta^3(\mathbf{x}-\mathbf{y}) \\
= -CC'(k^0 - k'^0) \int \mathrm{d}^3x & e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} \\
= -CC'(k^0 - k'^0) & e^{i(k^0+k'^0)\cdot\mathbf{x}}\delta^3(\mathbf{k}-\mathbf{k}') \\
= 0 &
\end{aligned} \tag{11}
$$

In the last step, we use the fact that $k^0 = k'^0$. Similarly, we find that

$$\left[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = 0 \tag{12}$$

$$\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = \delta^3(\mathbf{k} - \mathbf{k}') \tag{13}$$

So the creation and annihilation operators commute with themselves for any two $\mathbf{k}$ and $\mathbf{k}'$, but do not commute with each other.

2.2 Relationship with the Harmonic Oscillator

The Hamiltonian is the integral of the Hamiltonian density $\mathcal{H}$ over all space:

$$\begin{aligned} H &= \int \mathrm{d}^3x \;\; \mathcal{H} \\ &= \frac{1}{2}\int \mathrm{d}^3x \Big(m^2\phi^2 + (\boldsymbol{\nabla}\phi)\cdot(\boldsymbol{\nabla}\phi) + \Pi^2 \Big) \end{aligned} \tag{14}$$

Recall that $k^0 = k'^0$. Using equation 1:

$$\begin{aligned} \int \mathrm{d}^3x \;\; \phi^2(\mathbf{x}) = &\frac{1}{2(2\pi)^3}\int \mathrm{d}^3x \iint \frac{\mathrm{d}^3k}{\sqrt{k^0}}\frac{\mathrm{d}^3k'}{\sqrt{k'^0}} \Big(e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} a(\mathbf{k})a(\mathbf{k}') \\ &+ e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} a(\mathbf{k})a^\dagger(\mathbf{k}') + e^{-i(-\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} a^\dagger(\mathbf{k})a(\mathbf{k}') \\ &+ e^{-i(-\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} a^\dagger(\mathbf{k})a^\dagger(\mathbf{k}') \Big) \\ = \frac{1}{2}\iint &\frac{\mathrm{d}^3k}{\sqrt{k^0}}\frac{\mathrm{d}^3k'}{\sqrt{k'^0}} \Big(e^{-i(k^0+k'^0)x^0} a(\mathbf{k})a(\mathbf{k}')\delta^3(\mathbf{k}+\mathbf{k}') \\ &+ e^{-i(k^0-k'^0)x^0} a(\mathbf{k})a^\dagger(\mathbf{k}')\delta^3(\mathbf{k}-\mathbf{k}') + e^{-i(-k^0+k'^0)x^0} a^\dagger(\mathbf{k})a(\mathbf{k}')\delta^3(-\mathbf{k}+\mathbf{k}') \\ &+ e^{-i(-k^0-k'^0)x^0} a^\dagger(\mathbf{k})a^\dagger(\mathbf{k}')\delta^3(-\mathbf{k}-\mathbf{k}') \Big) \\ = \frac{1}{2k^0}\int &\mathrm{d}^3k \;\; \Big(e^{-2ik^0x^0} a(\mathbf{k})a(-\mathbf{k}) + e^0 a(\mathbf{k})a^\dagger(\mathbf{k}) \\ &+ e^0 a^\dagger(\mathbf{k})a(\mathbf{k}) + e^{2ik^0x^0} a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) \Big) \\ = \frac{1}{2k^0}\int &\mathrm{d}^3k \;\; \Big(e^{-2ik^0x^0} a(\mathbf{k})a(-\mathbf{k}) + a(\mathbf{k})a^\dagger(\mathbf{k}) \\ &+ a^\dagger(\mathbf{k})a(\mathbf{k}) + e^{2ik^0x^0} a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) \Big) \end{aligned} \tag{15}$$

Similarly, using equation 5:

$$\int \mathrm{d}^3x \;\; \Pi^2(\mathbf{x}) = -\frac{1}{2(2\pi)^3}\int \mathrm{d}^3x \iint \mathrm{d}^3k \;\; \mathrm{d}^3k' \;\; \sqrt{k^0k'^0}\Big(e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}a(\mathbf{k})a(\mathbf{k}')$$
$$- e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}a(\mathbf{k})a^\dagger(\mathbf{k}') - e^{-i(-\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}a^\dagger(\mathbf{k})a(\mathbf{k}')$$
$$+ e^{-i(-\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}a^\dagger(\mathbf{k})a^\dagger(\mathbf{k}')\Big)$$
$$= -\frac{(k^0)^2}{2k^0}\int \mathrm{d}^3k \;\; \Big(e^{-2ik^0x^0}a(\mathbf{k})a(-\mathbf{k}) - a(\mathbf{k})a^\dagger(\mathbf{k})$$
$$- a^\dagger(\mathbf{k})a(\mathbf{k}) + e^{2ik^0x^0}a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})\Big) \tag{16}$$

The gradient of ϕ is found from equation 1:

$$\boldsymbol{\nabla}\phi(\mathbf{x}) = -iC\mathbf{k}\int \mathrm{d}^3k \;\; \Big(e^{(-i\mathbf{k}\cdot\mathbf{x})}a(\mathbf{k}) - e^{(i\mathbf{k}\cdot\mathbf{x})}a^\dagger(\mathbf{k})\Big) \tag{17}$$

So, we see that

$$\int \mathrm{d}^3x \;\; \boldsymbol{\nabla}\phi(\mathbf{x})\cdot\boldsymbol{\nabla}\phi(\mathbf{x}) = \frac{(i)^2}{2(2\pi)^3}\int \mathrm{d}^3x \iint \frac{\mathrm{d}^3k}{\sqrt{k^0}}\frac{\mathrm{d}^3k'}{\sqrt{k'^0}}\mathbf{k}$$
$$\cdot\,\mathbf{k}'\Big(e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}a(\mathbf{k})a(\mathbf{k}') - e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}a(\mathbf{k})a^\dagger(\mathbf{k}')$$
$$- e^{-i(-\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}a^\dagger(\mathbf{k})a(\mathbf{k}') + e^{-i(-\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}a^\dagger(\mathbf{k})a^\dagger(\mathbf{k}')\Big)$$
$$= \frac{\mathbf{k}^2}{2k^0}\int \mathrm{d}^3k \;\; \Big(e^{-2ik^0x^0}a(\mathbf{k})a(-\mathbf{k}) + a(\mathbf{k})a^\dagger(\mathbf{k})$$
$$+ a^\dagger(\mathbf{k})a(\mathbf{k}) + e^{2ik^0x^0}a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})\Big) \tag{18}$$

Substituting equations 2.2, 2.2, and 2.2 into equation 14, we can derive an equation for the Hamiltonian:

$$H = \frac{1}{4k^0}\int \mathrm{d}^3k \;\; \Big[(m^2+\mathbf{k}^2-(k^0)^2)\Big(e^{-2ik^0x^0}a(\mathbf{k})a(-\mathbf{k})$$
$$+ e^{2ik^0x^0}a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})\Big) + (m^2+\mathbf{k}^2+(k^0)^2)\Big(a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k})\Big)\Big]$$
$$= \frac{1}{4k^0}\int \mathrm{d}^3k \;\; \Big[0\times\Big(e^{-2ik^0x^0}a(\mathbf{k})a(-\mathbf{k})$$
$$+ e^{2ik^0x^0}a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})\Big) + 2(k^0)^2\Big(a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k})\Big)\Big]$$

$$= \frac{1}{2}\int \mathrm{d}^3k \;\; k^0 \Big(a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k}) \Big)$$
$$= \frac{1}{2}\int \mathrm{d}^3k \;\; E_k \Big(a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k}) \Big) \tag{19}$$

Recalling the commutation relations from equations 2.1, 12, and 13, the commutation relations of the annihilation and creation operators with the Hamiltonian are easily calculated to be

$$[a(\mathbf{k}), H] = E_k a(\mathbf{k}) \tag{20}$$
$$\left[a^\dagger(\mathbf{k}), H\right] = -E_k a^\dagger(\mathbf{k}) \tag{21}$$

So the annihilation and creation operators annihilate and create a quantum of energy E_k, respectively. This is identical in form to the harmonic oscillator. Equations 20 and 21 therefore naturally lead to the description of the Klein-Gordon field as an infinite set of uncoupled harmonic oscillators, one for each point in space-time $\mathbf{x}$.

2.3 Normal Ordering

The problem with the harmonic oscillator description of the Klein-Gordon field is that harmonic oscillators have nonzero ground state energy due to an additive constant. Clearly, a system consisting of an infinite number of such oscillators will have infinite energy in its ground state alone, which is nonphysical. The way around this thorny issue is to take advantage of the fact that the infinite energy comes from an additive constant, and simply shift the energy scale down to make the ground state have zero energy. We accomplish this by imposing the normal order: ordering the annihilation and creation operators a and $a^\dagger$ such that $a^\dagger$ is always left of a. It is denoted by a superscript $N.O.$ or surrounding colons.

$$\Big(aa^\dagger \Big)^{N.O.} =: aa^\dagger := a^\dagger a$$

The normal-ordered Hamiltonian is

$$H^{N.O.} = \frac{1}{2}\int \mathrm{d}^3k \;\; E_k \Big(: a(\mathbf{k})a^\dagger(\mathbf{k}) : + : a^\dagger(\mathbf{k})a(\mathbf{k}) : \Big)$$
$$= \int \mathrm{d}^3k \;\; E_k a^\dagger(\mathbf{k})a(\mathbf{k}) \tag{22}$$
$$= \int \mathrm{d}^3k \;\; E_k N(k) \tag{23}$$

where the number operator $N(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k})$. The total number operator is

$$N = \int d^3k N(\mathbf{k}) \tag{24}$$

The commutator relations follow easily:

$$\begin{aligned}
[a(\mathbf{k}), N(\mathbf{k}')] &= \left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] a(\mathbf{k}) \\
&= \delta^3(\mathbf{k} - \mathbf{k}')a(\mathbf{k}) && (25) \\
[a(\mathbf{k}), N] &= a(\mathbf{k}) && (26) \\
\left[a^\dagger(\mathbf{k}), N(\mathbf{k}')\right] &= a^\dagger(\mathbf{k})\left[a^\dagger(\mathbf{k}), a(\mathbf{k}')\right] \\
&= -\delta^3(\mathbf{k} - \mathbf{k}')a^\dagger(\mathbf{k}) && (27) \\
\left[a^\dagger(\mathbf{k}), N\right] &= -a^\dagger(\mathbf{k}) && (28)
\end{aligned}$$

2.4 Operations on Eigenstates

Consider an energy eigenstate $|E\rangle$. We would like to see how the annihilation and creation operators interact with the Hamiltonian on this eigenstate. Applying the commutator of a and H to $|E\rangle$, we obtain

$$\begin{aligned}
[a(\mathbf{k}), H] |E\rangle &= E_k a(\mathbf{k}) |E\rangle \\
-Ha(\mathbf{k}) |E\rangle &= E_k a(\mathbf{k}) |E\rangle - a(\mathbf{k})H |E\rangle \\
H(a(\mathbf{k}) |E\rangle) &= (E - E_k)(a(\mathbf{k}) |E\rangle) && (29)
\end{aligned}$$

using the fact that $H|E\rangle = E|E\rangle$. Similarly,

$$\begin{aligned}
\left[a^\dagger(\mathbf{k}), H\right] |E\rangle &= E_k a^\dagger(\mathbf{k}) |E\rangle \\
H(a^\dagger(\mathbf{k}) |E\rangle) &= (E + E_k)(a^\dagger(\mathbf{k}) |E\rangle) && (30)
\end{aligned}$$

So annihilation lowers the energy of the system by E_k and creation raises the energy by E_k. Since the ground state of the system has zero energy, the energy must be nonnegative. So, there must exist a minimum energy state $|E_{min}\rangle$ such that

$$a(\mathbf{k}) |E_{min}\rangle = 0$$

Define $|0\rangle \equiv |E_{min}\rangle$. The ground state is such that $H|0\rangle = N|0\rangle = 0$. Consider a one-particle state with nonzero energy:

$$|k\rangle = a^\dagger(\mathbf{k}) |0\rangle \tag{31}$$

We can construct any higher state in a similar way: with repeated applications of the creation operator. With normalization, these higher states can be formed by

$$|\Xi\rangle = \frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} |0\rangle \tag{32}$$

where there are n_i particles with momentum $\mathbf{k_i}$. It is clear that there should be $\sum_{i=1}^{l} n_i$ particles in this state, so

$$N|\Xi\rangle = (n_1 + n_2 + \cdots + n_l)|\Xi\rangle \tag{33}$$

Moreover, using the identity $[A, B^n] = \sum_{i=0}^{n-1} B^{n-i-1}[A,B]B^i$ and equation 13, we can see that there are indeed n_i particles with momentum $\mathbf{k_i}$, as we expect.

$$\begin{aligned}
\big[N(\mathbf{k}), (a^\dagger(\mathbf{k_j}))^{n_j}\big] &= a^\dagger(\mathbf{k})\big[a(\mathbf{k}), (a^\dagger(\mathbf{k_j}))^{n_j}\big] \\
&= a^\dagger(\mathbf{k}) \sum_{i=0}^{n_j-1} (a^\dagger(\mathbf{k_j}))^{n_j-i-1}\big[a(\mathbf{k}), a^\dagger(\mathbf{k_j})\big](a^\dagger(\mathbf{k_j}))^i \\
&= a^\dagger(\mathbf{k}) \sum_{i=0}^{n_j-1} (a^\dagger(\mathbf{k_j}))^{n_j-1}\delta^3(\mathbf{k}-\mathbf{k_j}) \\
&= n_j (a^\dagger(\mathbf{k_j}))^{n_j}\delta^3(\mathbf{k}-\mathbf{k_j})
\end{aligned} \tag{34}$$

$$\begin{aligned}
N(\mathbf{k})|\Xi\rangle &= N(\mathbf{k})\frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} |0\rangle \\
&= \frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \Big(n_1\delta^3(\mathbf{k}-\mathbf{k_1}) + N(\mathbf{k})\Big) \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} |0\rangle \\
&= \frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \Big(n_1\delta^3(\mathbf{k}-\mathbf{k_1}) + n_2\delta^3(\mathbf{k}-\mathbf{k_2}) + N(\mathbf{k})\Big) \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} |0\rangle \\
&= \frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} \Big(n_1\delta^3(\mathbf{k}-\mathbf{k_1}) \\
&\quad + n_2\delta^3(\mathbf{k}-\mathbf{k_2}) + \cdots + n_l\delta^3(\mathbf{k}-\mathbf{k_l}) + N(\mathbf{k})\Big)|0\rangle \\
&= \frac{(a^\dagger(\mathbf{k_1}))^{n_1}}{\sqrt{n_1!}} \frac{(a^\dagger(\mathbf{k_2}))^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a^\dagger(\mathbf{k_l}))^{n_l}}{\sqrt{n_l!}} \Big(n_1\delta^3(\mathbf{k}-\mathbf{k_1}) \\
&\quad + n_2\delta^3(\mathbf{k}-\mathbf{k_2}) + \cdots + n_l\delta^3(\mathbf{k}-\mathbf{k_l}))\Big)|0\rangle
\end{aligned} \tag{35}$$

We can also introduce a momentum operator

$$\mathbf{P} = \int \mathrm{d}^3k \;\; \mathbf{k}N(\mathbf{k}) \tag{36}$$

The actions of the Hamiltonian and momentum operators on our state $|\Xi\rangle$ can be determined easily from equations 35:

$$\begin{aligned} H\,|\Xi\rangle &= \int \mathrm{d}^3k E_k N(\mathbf{k})\,|\Xi\rangle \\ &= \sum_{i=1}^{l} n_i E_{k_i}\,|\Xi\rangle \end{aligned} \tag{37}$$

$$\begin{aligned} \mathbf{P}\,|\Xi\rangle &= \int \mathrm{d}^3k \mathbf{k} N(\mathbf{k})\,|\Xi\rangle \\ &= \sum_{i=1}^{l} n_i \mathbf{k_i}\,|\Xi\rangle \end{aligned} \tag{38}$$

The energy and momentum of the state, the eigenvalues of the Hamiltonian and momentum operators, are simply the sum of the energies and momenta of all of the particles in the state.

Consider the state in equation 14, $|k\rangle$. This represents a one particle state with four-momentum $k^\mu = (E_k, \mathbf{k})$. Clearly,

$$\begin{aligned} N\,|k\rangle &= |k\rangle \\ H\,|k\rangle &= E_k\,|k\rangle \\ \mathbf{P}\,|k\rangle &= \mathbf{k}\,|k\rangle \end{aligned} \tag{39}$$

In a similar way, we can apply the field operator itself to the ground state:

$$|\phi(\mathbf{x})\rangle = \phi(\mathbf{x})\,|0\rangle = \phi^{(-)}(\mathbf{x})\,|0\rangle \tag{40}$$

The $phi^{(+)}$ term is zero because it involves a and not $a^\dagger$ (equation 4). The projection onto $|\phi\rangle$ onto $|k\rangle$ is $\langle k|\phi(\mathbf{x})\rangle$. This projection is a solution to the Klein-Gordon equation, just like ϕ itself:

$$\begin{aligned} (\partial_\mu \partial^\mu + m^2)\,\langle k|\phi(\mathbf{x})\rangle &= \langle k|(\partial_\mu \partial^\mu + m^2)\phi(\mathbf{x})|0\rangle \\ &= 0\,\langle k|0\rangle \\ &= 0 \end{aligned} \tag{41}$$

So $\langle k|\phi(\mathbf{x})\rangle$ has a relation to the solutions of the Klein-Gordon equation. What is this relation? We proceed by calculating $\langle \phi(\mathbf{x})|k\rangle = \langle k|\phi(\mathbf{x})\rangle^*$.

$$\begin{aligned}
\langle \phi(\mathbf{x})|k\rangle &= \langle 0|a(\mathbf{k})\phi^{(-)}(\mathbf{x})|0\rangle^* \\
&= \left(C' \int \mathrm{d}^3k' \;\; e^{i\mathbf{k}'\cdot\mathbf{x}} \langle 0|a(\mathbf{k})a^\dagger(\mathbf{k}')|0\rangle \right)^* \\
&= C' \int \mathrm{d}^3k' \;\; e^{-i\mathbf{k}'\cdot\mathbf{x}} \Big(\langle 0|a^\dagger(\mathbf{k}')a(\mathbf{k})|0\rangle + \langle 0|[a(\mathbf{k}), a]^\dagger(\mathbf{k}')|0\rangle \Big) \\
&= C' \int \mathrm{d}^3k' \;\; e^{-i\mathbf{k}'\cdot\mathbf{x}} \delta^3(\mathbf{k}-\mathbf{k}') \\
&= Ce^{-i\mathbf{k}\cdot\mathbf{x}}
\end{aligned} \tag{42}$$

This is recognized as the plane-wave solution of the Klein-Gordon equation in the first quantization, connecting the two quantizations. Note that the probability of the system being in the state $|k\rangle$ is

$$\begin{aligned}
|\langle k|\phi(\mathbf{x})\rangle|^2 &= \langle k|\phi(\mathbf{x})\rangle \langle \phi(\mathbf{x})|k\rangle \\
&= C^2 \geq 0
\end{aligned} \tag{43}$$

since $k_0 = E_k > 0$. The probability for any composite state can also be found to be nonnegative.

3 Conclusion

Framing the Klein-Gordon equation within quantum field theory results in the second quantization. As we have seen, the field can be described as an infinite set of uncoupled oscillators, one for each point in space-time. Moreover, the probabilities to be in any state and the energies of those states are all nonnegative. In this way, the second quantization of the Klein-Gordon avoids many of the issues that plague the first quantization.

References

[1] Das A. 2008. *Lectures on Quantum Field Theory.* Hackensack, NJ: World Scientific Publishing.