Quantization of a Free Scalar Field

Consider the free scalar field with Lagrangian density

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

that we considered before. ϕ satisfies the Klein-Gordon equation

$$(\Box + m^2)\phi = 0 \quad \leftarrow \text{ This has solutions } e^{\pm i k \cdot x}$$

$k \cdot x \equiv k_\mu x^\mu$

$k^\mu = (E(\vec{k}), \vec{k})$

$k_\mu = \eta_{\mu\nu} k^\nu = (E(\vec{k}), -\vec{k})$

The Hamiltonian density is

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}(\vec{\nabla}\phi)^2 + \frac{1}{2} m^2 \phi^2$$

The general solution of the Klein-Gordon equation is

$$\phi(x) = \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \left[a(\vec{k}) e^{-ik\cdot x} + a^*(\vec{k}) e^{ik\cdot x} \right]$$

Then

$$\pi(x) = \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \left[-iE(\vec{k}) \right] \left[a(\vec{k}) e^{-ik\cdot x} - a^*(\vec{k}) e^{ik\cdot x} \right]$$

To quantize the field, we follow the usual canonical procedure:

$$\{\phi, \pi\} \longrightarrow i[\hat{\phi}, \hat{\pi}]$$

$$a(\vec{k}) \longrightarrow \hat{a}(k)$$

$$a^*(\vec{k}) \longrightarrow \hat{a}^\dagger(k)$$

In particular, we impose

$$[\hat{\phi}(\vec{x},t), \hat{\pi}(\vec{x}',t)] = i\,\delta^{(3)}(\vec{x}-\vec{x}')$$

What does this imply about $[\hat{a}(k), \hat{a}^\dagger(\vec{k}')]$?

To answer this question, compute

$$\hat{\phi}(\vec{x},t)\,\hat{\pi}(\vec{x}',t)$$

$$= \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \left[\hat{a}(\vec{k}) e^{-iE(\vec{k})t} e^{i\vec{k}\cdot\vec{x}} + \hat{a}^\dagger(\vec{k}) e^{iE(\vec{k})t} e^{-i\vec{k}\cdot\vec{x}}\right]$$

$$\times (-i) \int \frac{d^3\vec{k}'}{(2\pi)^3} \frac{E(\vec{k}')}{\sqrt{2E(\vec{k}')}} \left[\hat{a}(\vec{k}') e^{-iE(\vec{k}')t} e^{i\vec{k}'\cdot\vec{x}'} - \hat{a}^\dagger(\vec{k}') e^{iE(\vec{k}')t} e^{-i\vec{k}'\cdot\vec{x}'}\right]$$

$$= -i \int \frac{d^3\vec{k}}{(2\pi)^3} \int \frac{d^3\vec{k}'}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \frac{E(\vec{k}')}{\sqrt{2E(\vec{k}')}}$$

$$\times \Big[\hat{a}(\vec{k})\hat{a}(\vec{k}') e^{-i[E(\vec{k})+E(\vec{k}')]t} e^{i\vec{k}\cdot\vec{x}} e^{i\vec{k}'\cdot\vec{x}'}$$

$$- \hat{a}(\vec{k})\hat{a}^\dagger(\vec{k}') e^{-i[E(\vec{k})-E(\vec{k}')]t} e^{i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\cdot\vec{x}'}$$

$$+ \hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}') e^{i[E(\vec{k})-E(\vec{k}')]t} e^{-i\vec{k}\cdot\vec{x}} e^{i\vec{k}'\cdot\vec{x}'}$$

$$- \hat{a}^\dagger(\vec{k})\, \hat{a}^\dagger(\vec{k}')\, e^{i[E(\vec{k}) + E(\vec{k}')]t}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'} \Big]$$

Now compute

$$\hat{\pi}(\vec{x}', t)\, \hat{\phi}(\vec{x}, t)$$

$$= (-i) \int \frac{d^3\vec{k}}{(2\pi)^3} \int \frac{d^3\vec{k}'}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \frac{E(\vec{k}')}{\sqrt{2E(\vec{k}')}}$$

$$\times \Big[\hat{a}(\vec{k}')\, \hat{a}(\vec{k})\, e^{-i[E(\vec{k}') + E(\vec{k})]t}\, e^{i\vec{k}'\cdot\vec{x}'}\, e^{i\vec{k}\cdot\vec{x}}$$

$$+ \hat{a}(\vec{k}')\, \hat{a}^\dagger(\vec{k})\, e^{-i[E(\vec{k}') - E(\vec{k})]t}\, e^{i\vec{k}'\cdot\vec{x}'}\, e^{-i\vec{k}\cdot\vec{x}}$$

$$- \hat{a}^\dagger(\vec{k}')\, \hat{a}(\vec{k})\, e^{i[E(\vec{k}') - E(\vec{k})]t}\, e^{-i\vec{k}'\cdot\vec{x}'}\, e^{i\vec{k}\cdot\vec{x}}$$

$$- \hat{a}^\dagger(\vec{k}')\, \hat{a}^\dagger(\vec{k})\, e^{i[E(\vec{k}') + E(\vec{k})]t}\, e^{-i\vec{k}'\cdot\vec{x}'}\, e^{-i\vec{k}\cdot\vec{x}} \Big]$$

Then

$$\hat{\phi}(\vec{x}, t)\, \hat{\pi}(\vec{x}', t) - \hat{\pi}(\vec{x}', t)\, \hat{\phi}(\vec{x}, t)$$

$$= -i \int \frac{d^3\vec{k}}{(2\pi)^3} \int \frac{d^3\vec{k}'}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \frac{E(\vec{k}')}{\sqrt{2E(\vec{k}')}}$$

$$\times \Big[- \hat{a}(\vec{k})\, \hat{a}^\dagger(\vec{k}')\, e^{-i[E(\vec{k}) - E(\vec{k}')]t}\, e^{i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'} \qquad (1)$$

$$+ \hat{a}^\dagger(\vec{k})\, \hat{a}(\vec{k}')\, e^{i[E(\vec{k}) - E(\vec{k}')]t}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{i\vec{k}'\cdot\vec{x}'} \qquad (2)$$

$$- \hat{a}(\vec{k}')\hat{a}^\dagger(\vec{k})e^{-i[E(\vec{k}')-E(\vec{k})]t}\, e^{i\vec{k}'\cdot\vec{x}'}\, e^{-i\vec{k}\cdot\vec{x}} \qquad ③$$

$$+ \hat{a}^\dagger(\vec{k}')\hat{a}(\vec{k})e^{i[E(\vec{k}')-E(\vec{k})]t}\, e^{-i\vec{k}'\cdot\vec{x}'}\, e^{i\vec{k}\cdot\vec{x}} \Big] \qquad ④$$

If

$$[\hat{a}(\vec{k}), \hat{a}(\vec{k}')] = 0$$

$$[\hat{a}^\dagger(\vec{k}), \hat{a}^\dagger(\vec{k}')] = 0$$

Further, if

$$[\hat{a}(\vec{k}), \hat{a}^\dagger(\vec{k}')] = (2\pi)^3 \delta^{(3)}(\vec{k}-\vec{k}')$$

then

$$[\hat{\phi}(\vec{x},t), \hat{\pi}(\vec{x}',t)]$$

$$= i\int \frac{d^3\vec{k}}{(2\pi)^3}\int \frac{d^3\vec{k}'}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k}')}} \frac{E(\vec{k}')}{\sqrt{2E(\vec{k}')}}$$

$$\times \Big[(2\pi)^3\delta^{(3)}(\vec{k}-\vec{k}')\, e^{-i[E(\vec{k})-E(\vec{k}')]t}\, e^{i\vec{k}\cdot\vec{x}}\, e^{-i\vec{k}'\cdot\vec{x}'} \qquad ①+④$$

$$+(2\pi)^3\delta^{(3)}(\vec{k}'-\vec{k})\, e^{i[E(\vec{k})-E(\vec{k}')]t}\, e^{-i\vec{k}\cdot\vec{x}}\, e^{i\vec{k}'\cdot\vec{x}'}\Big] \qquad ③+②$$

$$= i\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{1}{2}\Big[e^{i\vec{k}\cdot(\vec{x}-\vec{x}')} + e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')}\Big] = i\,\delta^{(3)}(\vec{x}-\vec{x}')$$

Therefore, if we impose

$$[\hat{\phi}(\vec{x},t), \hat{\Pi}(\vec{x},t)] = i\,\delta^{(3)}(\vec{x}-\vec{x}\,')$$

then

$$[\hat{a}(\vec{k}), \hat{a}^{\dagger}(\vec{k}')] = (2\pi)^3\,\delta^{(3)}(\vec{k}-\vec{k}')$$

which is the commutation relation for the creation and annihilation operators of the harmonic oscillator!

HOMEWORK 1:

Derive the Hamiltonian for the real scalar field $\hat{\phi}$. Interpret the result. What is the number operator in this case?

Given the Hamiltonian, show that $\hat{\phi}$ satisfies the Heisenberg equations of motion.

Derive the momentum operator for $\hat{\phi}$. Interpret the result.

The above homework problems will further suggest the interpretation of $\hat{a}(\vec{k})$ and $\hat{a}^{\dagger}(\vec{k})$ as annihilation and creation operators, respectively, of particles (in this case scalar, spin 0, particles) of momentum $\vec{k}$ – i.e., of quanta in mode $\vec{k}$ of the quantized field $\hat{\phi}$.

The action of $\hat{a}(\vec{k})$ and $\hat{a}^{\dagger}(\vec{k})$ on the vacuum are

$$\sqrt{2E(\vec{k})}\,\hat{a}(\vec{k})\,|0\rangle = 0 \qquad (\text{this is the same as } \hat{a}(\vec{k})|0\rangle = 0)$$

$$\sqrt{2E(\vec{k})}\, \hat{a}^{\dagger}(\vec{k})\,|0\rangle = |\vec{k}\rangle$$

The factor $\sqrt{2E(\vec{k})}$ is a convenient relativistic normalization.

To develop a better understanding of the quantized scalar field operator, let's compute

$$\langle \vec{p}\,|\,\hat{\phi}(x)\,|0\rangle$$

$$= \langle 0|\sqrt{2E(\vec{p})}\,\hat{a}(\vec{p}) \int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{2E(\vec{k})}}\left[\hat{a}(\vec{k})e^{-ik\cdot x} + \hat{a}^{\dagger}(\vec{k})e^{ik\cdot x}\right]|0\rangle$$

$$= \int \frac{d^3k}{(2\pi)^3}\left[\frac{2E(\vec{p})}{2E(\vec{k})}\right]^{1/2} e^{ik\cdot x}\,\langle 0|\hat{a}(\vec{p})\,\hat{a}^{\dagger}(\vec{k})|0\rangle$$

$$= \int \frac{d^3k}{(2\pi)^3}\left[\frac{2E(\vec{p})}{2E(\vec{k})}\right]^{1/2} e^{ik\cdot x}\,\langle 0|\left[\hat{a}^{\dagger}(\vec{k})\,\hat{a}(\vec{p}) + 2\pi\,\delta^{(3)}(\vec{k}-\vec{p})\right]|0\rangle$$

$$= \int d^3k\left[\frac{2E(\vec{p})}{2E(\vec{k})}\right]^{1/2} e^{ik\cdot x}\,\delta^{(3)}(\vec{k}-\vec{p})\,\underbrace{\langle 0|0\rangle}_{\equiv 1}$$

$$= e^{ip\cdot x}$$

$$= e^{iE(\vec{p})t}\,e^{-i\vec{p}\cdot\vec{x}}$$

$$= e^{iE(\vec{p})t}\,\langle \vec{p}\,|\,\vec{x}\rangle$$

Thus

$$\hat{\phi}(x)\,|0\rangle = e^{iE(\vec{p})t}\,|\vec{x}\rangle$$

- i.e., the operator creates a free spin-0 particle of mass m and energy $E(\vec{p})$ (momentum $\vec{p}$) at $\vec{x}$ (i.e., in the position eigenstate $|\vec{x}\rangle$).

Since $\hat{\phi}(x)$ is Hermitian

$$\hat{\phi}^\dagger(x) = \hat{\phi}(x)$$

We have

$$\langle x| = (|x\rangle)^\dagger = (\hat{\phi}(x)|0\rangle)^\dagger = \langle 0|\hat{\phi}^\dagger(x) = \langle 0|\hat{\phi}(x)$$

Then the wave function of a particle in state $|\psi\rangle$ is

$$\psi(x) = \langle x|\psi\rangle = \langle 0|\hat{\phi}(x)|\psi\rangle$$

Let's consider the time evolution of $\psi(x)$

$$\partial_t \psi(x) = \partial_t \langle 0|\hat{\phi}(x)|\psi\rangle$$

$$= \langle 0|\partial_t \hat{\phi}(x)|\psi\rangle$$

$$= \langle 0|\int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{2E(\vec{k})}}\left[-iE(\vec{k})\right]\left[\hat{a}(\vec{k})e^{-ik\cdot x} - \hat{a}^\dagger(\vec{k})e^{ik\cdot x}\right]|\psi\rangle$$

$$= -i \langle 0 | \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2E(\vec{k})}} \left[\vec{k}^2 + m^2\right]^{1/2} \left[\hat{a}(\vec{k}) e^{-ik\cdot x} - \hat{a}^\dagger(\vec{k}) e^{ik\cdot x}\right] | \psi \rangle$$

$$= -i \langle 0 | \left[-\vec{\nabla}^2 + m^2\right]^{1/2} \hat{\phi}(x) | \psi \rangle$$

$$= -i \left[-\vec{\nabla}^2 + m^2\right]^{1/2} \langle 0 | \hat{\phi}(x) | \psi \rangle$$

$$= -i \left[-\vec{\nabla}^2 + m^2\right]^{1/2} \psi(x)$$

$$= -i m \left[1 - \frac{1}{m^2} \vec{\nabla}^2\right]^{1/2} \psi(x)$$

$$\simeq -i m \left[1 - \frac{1}{2m^2} \vec{\nabla}^2\right] \psi(x)$$

Then

$$i \partial_t \psi \simeq \left(m - \frac{1}{2m} \nabla^2\right) \psi$$

$$= \left(\hat{H}_{\text{nonrelativistic}} + m\right) \psi$$

The term m (really mc^2) can be dropped. It contributes a constant to the overall Hamiltonian and does not affect the dynamics.

So, we have

$$i \partial_t \psi \simeq -\frac{1}{2m} \vec{\nabla}^2 \psi .$$

in the nonrelativistic limit, which is just Schrödinger's equation for the single free scalar particle in this limit.

Multi-Particle States and Fock Space

Using the creation operators, one can construct multiparticle states. For example, the following is a 2-particle state

$$\hat{a}^{+}(\vec{k}_1)\,\hat{a}^{+}(\vec{k}_2)\,|0\rangle = |\vec{k}_1\,\vec{k}_2\rangle$$

The possibilities are literally endless

$$|0\rangle,\ \underbrace{\hat{a}^{+}(\vec{k}_1)|0\rangle}_{|\vec{k}_1\rangle},\ \underbrace{\hat{a}^{+}(\vec{k}_1)\,\hat{a}^{+}(\vec{k}_2)|0\rangle}_{|\vec{k}_1\,\vec{k}_2\rangle},\ \underbrace{a^{+}(\vec{k}_1)\,a^{+}(\vec{k}_2)\,a^{+}(\vec{k}_3)|0\rangle}_{|\vec{k}_1\,\vec{k}_2\,\vec{k}_3\rangle},\ \ldots$$

The Hilbert space is a <u>direct sum</u> of n-particle Hilbert spaces ($n = 0, 1, 2, \ldots$)

$$\mathcal{F}_n = \bigoplus_n \mathcal{H}_n$$

known as <u>Fock Space</u>.

Let's look at some matrix elements (observables). Consider a two particle system with one particle in mode $\vec{k}_1$ and the other in mode $\vec{k}_2$.

Let's check that the number operator

$$\hat{N} = \int \frac{d^3\vec{k}}{(2\pi)^3}\, \hat{a}^\dagger(\vec{k})\,\hat{a}(\vec{k})$$

returns the number 2:

$$\langle \vec{k}_1 \vec{k}_2 | \hat{N} | \vec{k}_1 \vec{k}_2 \rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \int \frac{d^3\vec{k}}{(2\pi)^3}\, \hat{a}^\dagger(\vec{k})\,\hat{a}(\vec{k})\,\hat{a}^\dagger(\vec{k}_1)\,\hat{a}^\dagger(\vec{k}_2)|0\rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \int \frac{d^3\vec{k}}{(2\pi)^3} \Big[\hat{a}^\dagger(\vec{k})\,\hat{a}^\dagger(\vec{k}_1)\,\hat{a}(\vec{k})\,\hat{a}^\dagger(\vec{k}_2) + (2\pi)^3 \delta^{(3)}(\vec{k}-\vec{k}_1)\,\hat{a}^\dagger(\vec{k})\,\hat{a}^\dagger(\vec{k}_2) \Big] |0\rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \int \frac{d^3\vec{k}}{(2\pi)^3} \Big[\hat{a}^\dagger(\vec{k})\,\hat{a}^\dagger(\vec{k}_1)\,\hat{a}^\dagger(\vec{k}_2)\,\hat{a}(\vec{k}) + (2\pi)^3 \delta^{(3)}(\vec{k}-\vec{k}_2)\,\hat{a}^\dagger(\vec{k})\,\hat{a}^\dagger(\vec{k}_1) + (2\pi)^3 \delta^{(3)}(\vec{k}-\vec{k}_1)\,\hat{a}^\dagger(\vec{k})\,\hat{a}^\dagger(\vec{k}_2) \Big] |0\rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \hat{a}^\dagger(\vec{k}_2)\,\hat{a}^\dagger(\vec{k}_1)|0\rangle + \langle \vec{k}_1 \vec{k}_2 | \hat{a}^\dagger(\vec{k}_1)\,\hat{a}^\dagger(\vec{k}_2)|0\rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \vec{k}_1 \vec{k}_2 \rangle + \langle \vec{k}_1 \vec{k}_2 | \vec{k}_2 \vec{k}_1 \rangle$$

$|\vec{k}_1 \vec{k}_2\rangle = |\vec{k}_2 \vec{k}_1\rangle$ for $[a(\vec{k}_1), a^\dagger(\vec{k}_2)] = 0$ – i.e., for bosons

$$= \langle \vec{k}_1 \vec{k}_2 | \vec{k}_1 \vec{k}_2 \rangle + \langle \vec{k}_1 \vec{k}_2 | \vec{k}_1 \vec{k}_2 \rangle$$

$$= 2$$

What about the total energy?

$$\langle \vec{k}_1 \vec{k}_2 | \hat{H} | \vec{k}_1 \vec{k}_2 \rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | \int \frac{d^3\vec{k}}{(2\pi)^3} E(\vec{k}) \left[\text{from page 12} \right] | 0 \rangle$$

$$= \langle \vec{k}_1 \vec{k}_2 | E(\vec{k}_2) a^\dagger(\vec{k}_2) a^\dagger(\vec{k}_1) | 0 \rangle$$

$$+ \langle \vec{k}_1 \vec{k}_2 | E(\vec{k}_1) a^\dagger(\vec{k}_1) a^\dagger(\vec{k}_2) | 0 \rangle$$

$$= E(\vec{k}_2) \langle \vec{k}_1 \vec{k}_2 | \vec{k}_1 \vec{k}_2 \rangle + E(\vec{k}_1) \langle \vec{k}_1 \vec{k}_2 | \vec{k}_2 \vec{k}_1 \rangle$$

$$= \left[E(\vec{k}_2) + E(\vec{k}_1) \right] \langle \vec{k}_1 \vec{k}_2 | \vec{k}_1 \vec{k}_2 \rangle$$

$$= E(\vec{k}_1) + E(\vec{k}_2)$$

as expected.

Note that the symmetry/antisymmetry associated with identical particles is built into the commutators.

For bosons:

$$|\vec{k}_1, \vec{k}_2\rangle = |\vec{k}_2, \vec{k}_1\rangle$$

But

$$|\vec{k}_1, \vec{k}_2\rangle = \hat{a}^\dagger(\vec{k}_2)\,\hat{a}^\dagger(\vec{k}_1)\,|0\rangle$$

$$|\vec{k}_2, \vec{k}_1\rangle = a^\dagger(\vec{k}_1)\,\hat{a}^\dagger(\vec{k}_2)\,|0\rangle$$

Given that

$$[\hat{a}^\dagger(\vec{k}_1), \hat{a}^\dagger(\vec{k}_2)] = 0$$

for bosons, it is easy to see that

$$|\vec{k}_1, \vec{k}_2\rangle = |\vec{k}_2, \vec{k}_1\rangle$$

For fermions, we will see that

$$\{\hat{a}^\dagger(\vec{k}_1), \hat{a}^\dagger(\vec{k}_2)\} = 0$$

which then gives

$$|\vec{k}_1, \vec{k}_2\rangle = -|\vec{k}_2, \vec{k}_1\rangle$$