2 Scalar Field Quantization

We will study canonical quantization of real scalar field.

2.1 Classical field Lagrangian and Hamiltonian

Klein-Gordon equation of free real scalar field $\phi(x)$ is

$$(\partial^2 + m^2)\phi(x) = 0 \tag{2.1}$$

It is derived from the Lagrangian, after applying into Euler-Lagrange equation, appear in the form

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 \tag{2.2}$$

For example

$$0 = \frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi} = -m^2\phi - \partial^2\phi$$

Its solution is derived as in the following

$$\phi(x) \propto a(k)e^{-ik\cdot x} \mapsto (-k^2 + m^2)a(k) = 0 \tag{2.3}$$

$$a(k) \neq 0 \mapsto 0 = -k^2 + m^2 = -\omega^2 + |\vec{k}|^2 + m^2 \text{ or } \omega^2 - \omega_k^2 = 0 \tag{2.4}$$

with $\omega_k = \sqrt{|\vec{k}|^2 + m^2}$. The general solution is

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3}\int\frac{d\omega}{2\pi}\left(a(k)e^{-ik\cdot x} + c.c.\right)(2\pi)\delta(\omega^2 - \omega_k^2) \tag{2.5}$$

From identity

$$\delta(f(x)) = \sum_i \frac{\delta(x - a_i)}{|f'(a_i)|}, \text{ where } f(a_i) = 0$$

$$\mapsto \delta(\omega^2 - \omega_k^2) = \frac{1}{2\omega_k}\left(\delta(\omega - \omega_k) + \delta(\omega + \omega_k)\right)$$

From (2.5), we have

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\left(a(k)e^{-ik\cdot x} + c.c.\right)_{\omega=\omega_k} \tag{2.6}$$

The conjugate momentum field $\pi(x)$ is derived to be in the form

$$\pi(x) = \frac{\partial\mathcal{L}}{\partial\partial_0\phi} = \partial_0\phi(x) \mapsto \partial_0\phi(x) = \pi(x) \tag{2.7}$$

The field Hamiltonian is derived from Legendre transformation of the Lagrangian as

$$\mathcal{H} = \pi\partial_0\phi - \mathcal{L} = \frac{1}{2}\pi^2 + \frac{1}{2}\nabla\phi\cdot\nabla\phi + \frac{1}{2}m^2\phi^2 \tag{2.8}$$

$$\mapsto H = \frac{1}{2}\int d^3x\left(\pi^2 + \nabla\phi\cdot\nabla\phi + m^2\phi^2\right) \tag{2.9}$$

Note from (2.6) that

$$\pi(x) = \partial_0\phi(x) = -\frac{i}{2}\int \frac{d^3k}{(2\pi)^3}\left(a(k)e^{-ik\cdot x} - a^*(k)e^{ik\cdot x}\right)_{\omega=\omega_k} \tag{2.10}$$

$$\nabla\phi(x) = i\int \frac{d^3k}{(2\pi)^3 2\omega_k}\vec{k}\left(a(k)e^{-ik\cdot x} - a^*(k)e^{ik\cdot x}\right)_{\omega=\omega_k} \tag{2.11}$$

The field amplitude is determined from the inverse Fourier transformation as

$$a(k) = \int d^3x e^{ik\cdot x}(\partial_0 - i\omega_k)\phi(x) \equiv \int d^3x e^{ik\cdot x}\overleftrightarrow{\partial}_0\phi(x) \tag{2.12}$$

$$a^*(k) = \int d^3x e^{-ik\cdot x}\overleftrightarrow{\partial}_0\phi(x) \tag{2.13}$$

After we have defined the notation $f\overleftrightarrow{\partial}_0 g = f(\partial_0 g) - (\partial_0 f)g$.

2.2 Canonical quantization

We promote the field $\phi(x)$ and its conjugate momentum field $\pi(x)$ to be quantum operators satisfy the *equal time commutation relation*

$$\begin{aligned} \phi(x) \mapsto \hat{\phi}(x),\ \pi(x) \mapsto \hat{\pi}(x) \\ \rightarrow [\hat{\phi}(x), \hat{\pi}(y)]_{x^0=y^0} = i\delta^{(3)}(\vec{x}-\vec{y}) \end{aligned} \tag{2.14}$$

From now on we will understand the field operators from the field without the hat. Let us study this commutation by insertion with (2.5) and (2.10), for convenient we will set $x^0 = y^0 = 0$, we have

$$\begin{aligned} [\phi(x), \pi(y)]_{x^0=y^0=0} &= -\frac{i}{2}\int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3} \\ &\quad \times \left[(a(k)e^{i\vec{k}\cdot\vec{x}} + a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}}), (a(k')e^{i\vec{k}'\cdot\vec{y}} - a^\dagger(k')e^{-i\vec{k}'\cdot\vec{y}})\right] \\ &= -\frac{i}{2}\int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3} \\ &\quad \times \Big\{[a(k), a(k')]e^{i\vec{k}\cdot\vec{x}+i\vec{k}'\cdot\vec{y}} - [a(k), a^\dagger(k')]e^{i\vec{k}\cdot\vec{k}-i\vec{k}'\cdot\vec{y}} \\ &\quad +[a^\dagger(k), a(k')]e^{-i\vec{k}\cdot\vec{x}+i\vec{k}'\cdot\vec{y}} - [a^\dagger(k), a^\dagger(k')]e^{-i\vec{k}\cdot\vec{x}-i\vec{k}'\cdot\vec{y}}\Big\} \end{aligned} \tag{2.15}$$

Let us assign the commutation relations

$$[a(k), a(k')] = 0 = [a^\dagger(k), a^\dagger(k')] \tag{2.16}$$

$$\left[a(k), a^\dagger(k')\right] = (2\pi)^3 2\omega_k\delta^{(3)}(\vec{k}-\vec{k}') \tag{2.17}$$

We will get from above

$$[\phi(x), \phi(y)]_{x^0=y^0=0} = i\int \frac{d^3k}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{x}-\vec{y})} = i\delta^{(3)}(\vec{x}-\vec{y}) \tag{2.18}$$

From this result we will get the field Hamiltonian operator, at $x^0 = y^0 = 0$, in the form

$$\begin{aligned}
H &= \frac{1}{2}\int d^3x \int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3 2\omega_{k'}} \\
&\quad \times \Big\{ -\omega_k\omega_{k'}\left(a(k)e^{i\vec{k}\cdot\vec{x}} - a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}}\right)\left(a(k')e^{i\vec{k}'\cdot\vec{x}} - a^\dagger(k')e^{-i\vec{k}'\cdot\vec{x}}\right) \\
&\quad -\vec{k}\cdot\vec{k'}\left(a(k)e^{i\vec{k}\cdot\vec{x}} - a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}}\right)\left(a(k')e^{i\vec{k}'\cdot\vec{x}} - a^\dagger(k')e^{-i\vec{k}'\cdot\vec{x}}\right) \\
&\quad +m^2\left(a(k)e^{i\vec{k}\cdot\vec{x}} + a^\dagger(k)e^{-i\vec{k}\cdot\vec{x}}\right)\left(a(k')e^{i\vec{k}'\cdot\vec{x}} + a^\dagger(k')e^{-i\vec{k}'\cdot\vec{x}}\right)\Big\} \\
&= \frac{1}{2}\int d^3x \int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3 2\omega_{k'}} \\
&\quad \times \Big\{(-\omega_k\omega_{k'} - \vec{k}\cdot\vec{k}' + m^2)\left[a(k)a(k')e^{i(\vec{k}+\vec{k}')\cdot\vec{x}} + a^\dagger(k)a^\dagger(k')e^{-i(\vec{k}+\vec{k}')\cdot\vec{x}}\right] \\
&\quad +(\omega_k\omega_{k'} + \vec{k}\cdot\vec{k}' + m^2)\left[a(k)a^\dagger(k')ei(\vec{k} - k")]\vec{)}\cdot\vec{c} + a^\dagger(k)a(k')e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}}\right]\Big\}
\end{aligned} \tag{2.19}$$

Apply the spatial integration

$$\int d^3x e^{\pm i(\vec{k}+\vec{k}')\cdot\vec{x}} = \delta^{(3)}(\vec{k}+\vec{k}') \mapsto \vec{k}' = -\vec{k}$$

$$\int d^3x e^{\pm i(\vec{k}-\vec{k}')\cdot\vec{x}} = \delta^{(3)}(\vec{k}-\vec{k}') \mapsto \vec{k}' = \vec{k}$$

After using the fact that

$$\vec{k}' = -\vec{k} \mapsto -\omega_k\omega_{k'} - \vec{k}\cdot\vec{k}' + m^2 = -\omega_k^2 + \vec{k}\cdot\vec{k} + m^2 = 0$$

$$\vec{k}' = \vec{k} \mapsto \omega_k\omega_{k'} + \vec{k}\cdot\vec{k}' + m^2 = \omega_k^2 + \vec{k}\cdot\vec{k} + m^2 = 2\omega_k^2$$

We will get field Hamiltonian operator from above, after doing momentum integration using delta function, in the form

$$\begin{aligned}
H &= \int \frac{d^3k}{(2\pi)^3 2\omega_k}\frac{\omega_k}{2}\left(a(k)a^\dagger(k) + a^\dagger(k)a(k)\right) \\
&= \int \frac{d^3k}{(2\pi)^3 2\omega_k}\omega_k\left(a^\dagger(k)a(k) + (2\pi)^3 2\omega_k\delta^{(3)}(0)\right)
\end{aligned} \tag{2.20}$$

The second part on the right hand side of (2.20) gives infinite result. To eliminate this part we define the *normal ordering* of field operator as

$$: aa^\dagger := a^\dagger a$$

And define the *vacuum state* $|0\rangle$ such that

$$a(k)|0\rangle = 0, \; a^\dagger(k) = |k\rangle \mapsto 1 - particle\ state$$

The physical Hamiltonian operator of quantized field is derived from (2.20) in the form

$$:H: = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\omega_k a^\dagger(k)a(k) \tag{2.21}$$

This shows that the quantum of real scalar field compose of a set of an infinite quantum harmonic oscillators, without vacuum energy. Note that the eliminated vacuum energy may play an importance role in *Casimir effect* of the quantum Universe which appear outside the context of quantum field theory.

2.3 Scalar field propagator

Let us determine the vacuum expectation value of commutator of two field operators

$$\begin{aligned}
i\Delta(x,y) = \langle 0|[\phi(x),\phi(y)]|0\rangle = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3 2\omega_{k'}} \\
\times\left\{\langle 0|[(a(k)e^{-ikx}+a^\dagger(k)e^{ikx}),(a(k')e^{-ik'y}+a^\dagger(k')e^{ik'y})]|0\rangle\right\} \\
= \int \frac{d^3k}{(2\pi)^3 2\omega_k}\int \frac{d^3k'}{(2\pi)^3 2\omega_{k'}}\left\{e^{-ikx+ik'y}\langle 0|[a(k),a^\dagger(k')]|0\rangle\right. \\
\left. +e^{ikx-ik'y}\langle 0|[a^\dagger(k),a(k')]|0\rangle\right\} \\
\mapsto i\Delta(x-y) = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\left\{e^{-ik(x-y)} - e^{ik(x-y)}\right\}
\end{aligned} \tag{2.22}$$

After we have used the commutation relation of field operators and doing $\int d^3k'$ integration using delta function.Let us changing the sign of $\vec{k}$ on the second term, we will have

$$i\Delta(x-y)\int \frac{d^3k}{(2\pi)^3 2\omega_k}e^{i\vec{k}\cdot(\vec{x}-\vec{y})}\left\{e^{-i\omega_k(x^0-y^0)} - e^{i\omega_k(x^0-y^0)}\right\} \tag{2.23}$$

Using identity

$$\frac{i}{\pi}\int d\omega \frac{e^{-i\omega(x^0-y^0)}}{\omega^2-\omega_k^2+i\epsilon} = \begin{cases} 1/\omega_k, & x^0-y^0>0 \\ -1/\omega_k, & x^0-y^0<0 \end{cases}$$

(This is determined from contour integration with Cauchy's theorem.) This result to

$$\begin{aligned}
i\Delta(x)-y) &= \int \frac{d^3k}{(2\pi)^3}\int \frac{d\omega}{2\pi}\frac{e^{-i\omega(x^0-y^0)+i\vec{k}\cdot(\vec{x}-\vec{y})}}{\omega^2-\omega_k^2+i\epsilon} \\
&= \int \frac{d^4k}{(2\pi)^4}\frac{e^{-ik\cdot(x-y)}}{k^2-m^2+i\epsilon},\ \text{when } k^2=\omega^2-\vec{k}^2 \qquad (2.24) \\
\mapsto i\Delta(k) &= \frac{1}{k^2-m^2+i\epsilon} \qquad (2.25)
\end{aligned}$$

On the other hand we can derive this expression from the vacuum expectation value of the *time-ordered* field operators as

$$\begin{aligned}\Delta_F(x-y) &= \langle 0|T[\phi(x)\phi(y)]|0\rangle \\ &= \theta(x^0-y^0)\langle 0|\phi(x)\phi(y)|0\rangle + \theta(y^0-x^0)\langle 0|\phi(y)\phi(x)|0\rangle \\ &= \int \frac{d^3k}{(2\pi)^3 2\omega_k} \int \frac{d^3k'}{(2\pi)^3 2\omega_{k'}} \langle 0|a(k)a^\dagger(k')|0\rangle e^{-ikx+ik'y} \\ &\qquad \times \left\{\theta(x^0-y^0)+\theta(y^0-x^0)\right\} \\ &= \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{-ik\cdot(x-y)} \left\{\theta(x^0-y^0)+\theta(y^0-x^0)\right\} \end{aligned} \tag{2.26}$$

After we have used the fact that $a(k)\ 0\rangle = 0$, $\langle 0|a^\dagger(k) = 0$, and used the commutation relation of the field operators $[a(k), a^\dagger(k')] = (2\pi)^3 2\omega_k \delta^{(3)}(k-k')$. Next after using the identity above we will get

$$\Delta_F(x-y) = -i\int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{e^{-ik\cdot(x-y)}}{\omega^2-\omega_k^2+i\epsilon} \tag{2.27}$$

$$\mapsto \Delta_F(k) = \frac{-i}{k^2-m^2+i\epsilon}, \text{ when } k^2 = \omega^2 - \vec{k}^2 \tag{2.28}$$

This is the same result as above.