1 Quantization of the Klein-Gordon (scalar) field

We develop the Hamiltonian formulation, then canonically quantize.

1.1 The conjugate momentum

To begin quantization, we require the Hamiltonian formulation of scalar field theory. Beginning with the Lagrangian,

$$L = \frac{1}{2} \int \left(\partial^{\alpha} \varphi \partial_{\alpha} \varphi - m^2 \varphi^2 \right) d^3 x$$

the only modification to the definition of the conjugate momentum as

$$p = \frac{\partial L}{\partial \dot{x}}$$

is the recognition that (a) the independent variable is dependent on four parameters $\varphi = \varphi(x^{\alpha})$ instead of just one, and (b) the Lagrangian is now a functional, Eq.(??). Just as the time derivative must be changed from a total to a partial derivative,

$$\dot{x} = \frac{dx}{dt} \Longrightarrow \dot{\varphi} = \frac{\partial \varphi}{\partial t}$$

the derivative of the Lagrangian must go to a functional derivative of the Lagrangian

$$\frac{\partial L}{\partial \dot{x}} \implies \frac{\delta L}{\delta \dot{\varphi}}$$

Writing $\pi(y^{\mu}) = \pi(y)$, the conjugate momentum is therefore,

$$\begin{aligned} \pi \left(y \right) &\equiv \frac{\delta L\left[x \right]}{\delta \left(\partial_0 \varphi \left(y \right) \right)} \\ &= \frac{\delta}{\delta \left(\partial_0 \varphi \left(y \right) \right)} \frac{1}{2} \int \left(\partial^\alpha \varphi \left(x \right) \partial_\alpha \varphi \left(x \right) - m^2 \varphi^2 \left(x \right) \right) d^3 x \\ &= \int \partial^0 \varphi \left(x \right) \delta^3 \left(\mathbf{y} - \mathbf{x} \right) d^3 x' \\ &= \partial^0 \varphi \left(t, \mathbf{y} \right) \end{aligned}$$

Notice that we treat $\varphi(\mathbf{x})$ and its derivatives $\partial_{\alpha}\varphi(\mathbf{x})$ as independent. In terms of the momentum density, the action and Lagrangian density are

$$S = \frac{1}{2} \int \left(\pi^2 - \nabla \varphi \cdot \nabla \varphi - m^2 \varphi^2 \right) d^4 x \tag{1}$$

$$\mathcal{L} = \frac{1}{2} \left(\pi^2 - \nabla \varphi \cdot \nabla \varphi - m^2 \varphi^2 \right)$$
(2)

1.2 The Hamiltonian and Poisson brackets

We must also generalize the expression for the Hamiltonian. For the infinite number of field degrees of freedom (labeled by the spatial coordinates \mathbf{x}), the sum in the expression for the Hamiltonian becomes an integral, so that $H = \sum p_i \dot{q}^i - L$ generalizes to

$$H = \int \pi (\mathbf{x}, t) \dot{\varphi} (\mathbf{x}, t) d^3 x - L$$
(3)

Therefore,

$$H = \int \pi(\mathbf{x})\dot{\varphi}(\mathbf{x})d^{3}x - \frac{1}{2}\int \left(\partial^{\alpha}\varphi\partial_{\alpha}\varphi - m^{2}\varphi^{2}\right)d^{3}x$$
$$= \frac{1}{2}\int \left(\pi^{2} + \nabla\varphi \cdot \nabla\varphi + m^{2}\varphi^{2}\right)d^{3}x \tag{4}$$

We can define the Hamiltonian density,

$$\mathcal{H} = \frac{1}{2} \left(\pi^2 + \boldsymbol{\nabla} \boldsymbol{\varphi} \cdot \boldsymbol{\nabla} \boldsymbol{\varphi} + m^2 \boldsymbol{\varphi}^2 \right)$$
(5)

Hamilton's equations can also be expressed in terms of densities. Starting from Hamilton's equations in the familiar form,

$$\begin{aligned} \dot{q}^i &=& \frac{\partial H}{\partial p_i} \\ \dot{p}_i &=& -\frac{\partial H}{\partial q^i} \end{aligned}$$

we replace (q^i, p_j) with (φ, π) and since the Hamiltonian is a functional, replace the partial derivative with functional derivatives,

$$\dot{\varphi}\left(\mathbf{x}\right) = \frac{\delta H}{\delta \pi\left(\mathbf{x}\right)} \tag{6}$$

$$\dot{\pi} \left(\mathbf{x} \right) = -\frac{\delta H}{\delta \varphi \left(\mathbf{x} \right)} \tag{7}$$

and check that our procedure reproduces the correct field equation by taking the indicated derivatives. Carrying out the functional derivative for $\dot{\varphi}$,

$$\begin{split} \dot{\varphi}(\mathbf{x}) &= \frac{\delta H}{\delta \pi_i \left(\mathbf{x}\right)} \\ &= \frac{1}{2} \frac{\delta}{\delta \pi_i \left(\mathbf{x}\right)} \int \left(\pi^2 + \nabla \varphi \cdot \nabla \varphi + m^2 \varphi^2\right) d^3 y \\ &= \frac{1}{2} \int \left(2\pi \left(\mathbf{y}\right) \frac{\delta \pi \left(\mathbf{y}\right)}{\delta \pi \left(\mathbf{x}\right)}\right) d^3 y \\ &= \int \pi \left(\mathbf{y}\right) \delta^3 \left(\mathbf{x} - \mathbf{y}\right) d^3 y \\ &= \pi \left(\mathbf{x}\right) \end{split}$$

This agrees with our definition of $\pi(\mathbf{x})$. For π we find

$$\begin{split} \dot{\pi} \left(\mathbf{x} \right) &= -\frac{\delta H}{\delta \varphi \left(\mathbf{x} \right)} \\ &= -\frac{1}{2} \frac{\delta}{\delta \varphi \left(\mathbf{x} \right)} \int \left(\pi^2 + \nabla \varphi \cdot \nabla \varphi + m^2 \varphi^2 \right) d^3 y \\ &= -\int \left(\nabla \varphi \cdot \nabla \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \varphi \left(\mathbf{x} \right)} + m^2 \varphi \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \varphi \left(\mathbf{x} \right)} \right) d^3 y \\ &= \int \left(\nabla^2 \varphi \cdot \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \varphi \left(\mathbf{x} \right)} - m^2 \varphi \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \varphi \left(\mathbf{x} \right)} \right) d^3 y \\ &= \int \left(\nabla^2 \varphi \delta^3 \left(\mathbf{y} - \mathbf{x} \right) - m^2 \varphi \delta^3 \left(\mathbf{y} - \mathbf{x} \right) \right) d^3 y \\ &= \nabla^2 \varphi \left(\mathbf{x} \right) - m^2 \varphi \left(\mathbf{x} \right) \end{split}$$

But $\dot{\pi} = \partial_0 \pi = \partial_0 \partial^0 \varphi$ so

$$\Box \varphi = -m^2 \varphi$$

and we recover the Klein-Gordon field equation.

We move toward quantization by writing the field equations in terms of functional Poisson brackets. Let

$$\{f(\varphi,\pi),g(\varphi,\pi)\} \equiv \int \left(\frac{\delta f}{\delta\pi(\mathbf{x})}\frac{\delta g}{\delta\varphi(\mathbf{x})} - \frac{\delta f}{\delta\varphi(\mathbf{x})}\frac{\delta g}{\delta\pi(\mathbf{x})}\right) d^3x \tag{8}$$

where we replace the sum over all p_i and q^i by an integral over \mathbf{x} , and where $f(\varphi, \pi) = f(\varphi(\mathbf{y}, t), \pi(\mathbf{y}, t))$ and $g(\varphi, \pi) = g(\varphi(\mathbf{z}, t), \pi(\mathbf{z}, t))$. The bracket is evaluated at a constant time. Then we have

$$\begin{aligned} \left\{ \pi \left(\mathbf{y}, t \right), \varphi \left(\mathbf{z}, t \right) \right\} &= \int \left(\frac{\delta \pi \left(\mathbf{y}, t \right)}{\delta \pi \left(\mathbf{x} \right)} \frac{\delta \varphi \left(\mathbf{z}, t \right)}{\delta \varphi \left(\mathbf{x} \right)} - \frac{\delta \pi \left(\mathbf{y}, t \right)}{\delta \varphi \left(\mathbf{x} \right)} \frac{\delta \varphi \left(\mathbf{z}, t \right)}{\delta \pi \left(\mathbf{x} \right)} \right) d^3 x \\ &= \int \delta^3 \left(\mathbf{y} - \mathbf{x} \right) \delta^3 \left(\mathbf{z} - \mathbf{x} \right) d^3 x \\ &= \delta^3 \left(\mathbf{z} - \mathbf{y} \right) \end{aligned}$$

while

$$\{\pi(\mathbf{y},t),\pi(\mathbf{z},t)\} = \{\varphi(\mathbf{y},t),\varphi(\mathbf{z},t)\} = 0$$

Hamilton's equations work out correctly:

$$\begin{split} \dot{\varphi}(\mathbf{x}) &= \{H(\varphi, \pi), \varphi(\mathbf{x}')\} \\ &= \int \left(\frac{\delta H(\varphi, \pi)}{\delta \pi(\mathbf{x})} \frac{\delta \varphi(\mathbf{x}')}{\delta \varphi(\mathbf{x})} - \frac{\delta H}{\delta \varphi(\mathbf{x})} \frac{\delta \varphi(\mathbf{x}')}{\delta \pi(\mathbf{x})}\right) d^3x \\ &= \int \frac{\delta H(\varphi, \pi)}{\delta \pi(\mathbf{x})} \delta^3(\mathbf{x} - \mathbf{x}') d^3x \\ &= \frac{\delta H(\varphi(\mathbf{x}), \pi(\mathbf{x}))}{\delta \pi(\mathbf{x})} \end{split}$$

and

$$\begin{split} \dot{\pi}(\mathbf{x}) &= \{H(\varphi, \pi), \pi(\mathbf{x}')\} \\ &= \int \left(\frac{\delta H(\varphi, \pi)}{\delta \pi(\mathbf{x})} \frac{\delta \pi(\mathbf{x}')}{\delta \varphi(\mathbf{x})} - \frac{\delta H}{\delta \varphi(\mathbf{x})} \frac{\delta \pi(\mathbf{x}')}{\delta \pi(\mathbf{x})}\right) d^3x \\ &= -\int \frac{\delta H(\varphi, \pi)}{\delta \varphi(\mathbf{x})} \delta^3(\mathbf{x} - \mathbf{x}') d^3x \\ &= -\frac{\delta H(\varphi(\mathbf{x}), \pi(\mathbf{x}))}{\delta \varphi(\mathbf{x})} \end{split}$$

Now we quantize, canonically. The field and its conjugate momentum become operators and the fundamental Poisson brackets become commutators:

$$\{\pi(\mathbf{x}'), \varphi(\mathbf{x}'')\} = \delta^3(\mathbf{x}'' - \mathbf{x}') \Rightarrow [\hat{\pi}(\mathbf{x}'), \hat{\varphi}(\mathbf{x}'')] = i\delta^3(\mathbf{x}'' - \mathbf{x}')$$

(where $\hbar = 1$) while

$$[\hat{\varphi}(\mathbf{x}'), \hat{\varphi}(\mathbf{x}'')] = [\hat{\pi}(\mathbf{x}'), \hat{\pi}(\mathbf{x}'')] = 0$$

These are the fundamental commutation relations of the quantum field theory. Because the commutator of the field operators $\hat{\pi}(\mathbf{x})$ and $\hat{\varphi}(\mathbf{x})$ are evaluated at the same value of t, these are called *equal time commutation* relations. More explicitly,

$$[\hat{\pi}(\mathbf{x}',t),\hat{\varphi}(\mathbf{x}'',t)] = i\delta^{3}(\mathbf{x}''-\mathbf{x}') [\hat{\varphi}(\mathbf{x}',t),\hat{\varphi}(\mathbf{x}'',t)] = [\hat{\pi}(\mathbf{x}',t),\hat{\pi}(\mathbf{x}'',t)] = 0$$

$$(9)$$

This completes the canonical quantization. The trick, of course, is to characterize the states these operators act on.

1.3 Solution for the free classical Klein-Gordon field

Having written commutation relations for the field, we still have the problem of finding solutions and interpreting them. To begin, we look at solutions the classical theory. The field equation

$$\Box \varphi \quad = \quad -\frac{m^2}{\hbar^2} \varphi$$

(where we keep \hbar , but set c = 1) is not hard to solve. Consider plane waves,

$$\begin{split} \varphi(\mathbf{x},t) &= Ae^{\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} + A^{\dagger}e^{-\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} \\ &= Ae^{\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{x})} + A^{\dagger}e^{-\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{x})} \end{split}$$

Substituting into the field equation we have

$$A\left(\frac{i}{\hbar}\right)^2 p_{\alpha} p^{\alpha} \exp \frac{i}{\hbar} \left(p_{\alpha} x^{\alpha}\right) = -\frac{m^2}{\hbar^2} A \exp \frac{i}{\hbar} \left(p_{\alpha} x^{\alpha}\right)$$

so we need the usual mass-energy-momentum relation:

$$p_{\alpha}p^{\alpha} = m^2$$

We can solve this for the energy,

$$E_{+} = \sqrt{\mathbf{p}^{2} + m^{2}}$$
$$E_{-} = -\sqrt{\mathbf{p}^{2} + m^{2}}$$

then construct the general solution by Fourier superposition. To keep the result manifestly relativistic, we use a Dirac delta function to impose the energy condition, $p_{\alpha}p^{\alpha} = m^2$. We also insert a unit step function, $\Theta(E)$, to insure positivity of the energy. This insertion may seem a bit *ad hoc*, and it is – we will save discussion of the negative energy solutions and antiparticles for the last section of this chapter. Then,

$$\varphi(\mathbf{x},t) = \frac{1}{(2\pi)^{3/2}} \int \sqrt{2E} \left(a(E,\mathbf{p}) e^{\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} + a^{\dagger}(E,\mathbf{p}) e^{-\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} \right) \\ \times \delta \left(p_{\alpha}p^{\alpha} - m^{2} \right) \Theta(E) \hbar^{-4} d^{4}p$$
(10)

where $A = \sqrt{2E}a(E, \mathbf{p})$ is the arbitrary complex amplitude of each wave mode and $\frac{1}{(2\pi)^{3/2}}$ is the conventional normalization for Fourier integrals.

Recall that for a function f(x) with zeros at x_i , i = 1, 2, ..., n, $\delta(f)$ gives a contribution at each zero:

$$\delta(f) = \sum_{i=1}^{n} \frac{1}{|f'(x_i)|} \delta(x - x_i)$$
(11)

so the quadratic delta function can be written as

$$\delta \left(p_{\alpha} p^{\alpha} - m^2 \right) = \delta \left(E^2 - \mathbf{p}^2 - m^2 \right)$$
$$= \frac{1}{2|E|} \delta \left(E - \sqrt{\mathbf{p}^2 + m^2} \right) + \frac{1}{2|E|} \delta \left(E + \sqrt{\mathbf{p}^2 + m^2} \right)$$

Exercise: Prove eq.(11).

Exercise: Argue that $\Theta(E)$ is Lorentz invariant.

The integral for the solution $\varphi(\mathbf{x}, t)$ becomes

$$\begin{split} \varphi(\mathbf{x},t) &= \frac{1}{(2\pi)^{3/2}} \int \sqrt{2E} \left\{ \left(ae^{\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} + a^{\dagger}e^{-\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} \right) \frac{1}{2|E|} \delta \left(E - \sqrt{\mathbf{p}^2 + m^2} \right) \right. \\ &+ \left(ae^{\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} + a^{\dagger}e^{-\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} \right) \frac{1}{2|E|} \delta \left(E + \sqrt{\mathbf{p}^2 + m^2} \right) \right\} \Theta(E)\hbar^{-4}d^4p \\ &= \frac{1}{(2\pi)^{3/2}} \int \left(ae^{\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} + a^{\dagger}e^{-\frac{i}{\hbar}(p_{\alpha}x^{\alpha})} \right) \frac{1}{\sqrt{2|E|}} \delta \left(E - \sqrt{\mathbf{p}^2 + m^2} \right) \hbar^{-4}d^4p \end{split}$$

Define the wave vector k^{μ} ,

$$k^{\mu} = (\omega, \mathbf{k})$$

$$\mathbf{k} = \frac{\mathbf{p}}{\hbar}$$

$$\omega = +\frac{1}{\hbar}\sqrt{\mathbf{p}^2 + m^2} = +\sqrt{\mathbf{k}^2 + \left(\frac{m}{\hbar}\right)^2}$$

Then integrating over the energy delta function,

$$\varphi\left(\mathbf{x},t\right) = \frac{1}{\left(2\pi\right)^{3/2}} \int \frac{d^3k}{\sqrt{2\omega}} \left(a\left(\mathbf{k}\right)e^{i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)} + a^{\dagger}\left(\mathbf{k}\right)e^{-i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)}\right)$$
(12)

This is the general classical solution for the Klein-Gordon field. Notice that since $\omega = \omega(\mathbf{k})$, the amplitudes a and a^{\dagger} depend only on \mathbf{k} . We also need the conjugate momentum,

$$\pi (\mathbf{x}, t) = \partial_0 \varphi (\mathbf{x}, t)$$

$$= \frac{i}{(2\pi)^{3/2}} \int d^3k \sqrt{\frac{\omega}{2}} \left(a \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - a^{\dagger} \left(\mathbf{k} \right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right)$$
(13)

To check that our solution satisfies the Klein-Gordon equation, we need only apply the wave operator to the right side. This pulls down an overall factor of $(ik_{\mu})(ik^{\mu}) = -\frac{1}{\hbar^2} (E^2 - \mathbf{p}^2) = -\frac{m^2}{\hbar^2}$. Since this is constant, it comes out of the integral, giving $-\frac{m^2}{\hbar^2}\varphi$ as required.

1.4 Quantization of the mode amplitudes

Now we need to quantize the classical *solution*. We know the fundamental commutation relations that $\hat{\varphi}$ and $\hat{\pi}$ satisfy, Eqs.(9) as operators, but we need to see the effect this has on the right hand side of the solution, Eq.(12). To do this, we first invert the classical Fourier integrals to solve for the coefficients in terms of the fields. To this end, multiply $\varphi(\mathbf{x},t)$ by $\frac{1}{(2\pi)^{3/2}}d^3xe^{i\mathbf{k'}\cdot\mathbf{x}}$ and integrate. It proves sufficient to evaluate the expression at t = 0.

$$\frac{1}{(2\pi)^{3/2}} \int \varphi\left(\mathbf{x},0\right) e^{i\mathbf{k}'\cdot\mathbf{x}} d^3x = \frac{1}{(2\pi)^3} \int \int \frac{d^3x d^3k}{\sqrt{2\omega}} \left(a\left(\mathbf{k}\right) e^{i\left(\mathbf{k}'-\mathbf{k}\right)\cdot\mathbf{x}} + a^{\dagger}\left(\mathbf{k}\right) e^{i\left(\mathbf{k}'+\mathbf{k}\right)\cdot\mathbf{x}}\right)$$
$$= \frac{1}{(2\pi)^3} \int \frac{d^3k}{\sqrt{2\omega}} \left(a\left(\mathbf{k}\right) (2\pi)^3 \delta^3\left(\mathbf{k}'-\mathbf{k}\right) + a^{\dagger}\left(\mathbf{k}\right) (2\pi)^3 \delta^3\left(\mathbf{k}'+\mathbf{k}\right)\right)$$
$$= \frac{1}{\sqrt{2\omega'}} \left(a\left(\mathbf{k}'\right) + a^{\dagger}\left(-\mathbf{k}'\right)\right)$$
(14)

where we have used the Fourier representation of the Dirac delta function

$$\frac{1}{\left(2\pi\right)^3}\int d^3x \ e^{i\mathbf{k}\cdot\mathbf{x}} = \delta^3(\mathbf{k})$$

Once again taking the Fourier transform, $\frac{1}{(2\pi)^{3/2}}\int \pi(\mathbf{x},0) e^{i\mathbf{k}'\cdot\mathbf{x}} d^3x$, of the momentum density, we find it equal to

$$\frac{1}{(2\pi)^{3/2}} \int \pi (\mathbf{x}, 0) e^{i\mathbf{k}' \cdot \mathbf{x}} d^3 x = \frac{i}{(2\pi)^3} \int d^3 x \int d^3 k \sqrt{\frac{\omega}{2}} \left(a (\mathbf{k}) e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}} - a^{\dagger} (\mathbf{k}) e^{i(\mathbf{k}' + \mathbf{k}) \cdot \mathbf{x}} \right)$$
$$= i \int d^3 k \sqrt{\frac{\omega}{2}} \left(a (\mathbf{k}) \delta^3 (\mathbf{k}' - \mathbf{k}) - a^{\dagger} (\mathbf{k}) \delta^3 (\mathbf{k}' + \mathbf{k}) \right)$$
$$= i \sqrt{\frac{\omega'}{2}} \left(a (\mathbf{k}') - a^{\dagger} (-\mathbf{k}') \right)$$
(15)

These results combine to solve for the amplitudes. Adding $\sqrt{2\omega'}$ times Eq.(14) to $-i\sqrt{\frac{2}{\omega'}}$ times (13) gives $a(\mathbf{k}')$:

$$\left(a\left(\mathbf{k}'\right) + a^{\dagger}\left(-\mathbf{k}'\right) \right) + \left(a(\mathbf{k}') - a^{\dagger}\left(-\mathbf{k}'\right) \right) = \frac{\sqrt{2\omega'}}{(2\pi)^{3/2}} \int \varphi\left(\mathbf{x},0\right) e^{i\mathbf{k}'\cdot\mathbf{x}} d^{3}x - \frac{i}{(2\pi)^{3/2}} \sqrt{\frac{2}{\omega'}} \int \pi\left(\mathbf{x},0\right) e^{i\mathbf{k}'\cdot\mathbf{x}} d^{3}x d^{3}x + \frac{i}{(2\pi)^{3/2}} \sqrt{\frac{2}{\omega'}} \int \pi\left(\mathbf{x},0\right) e^{i\mathbf{k}'\cdot\mathbf{x}} d^{3}x d^{3}$$

Simplifying, we have solve for the mode amplitudes,

$$a(\mathbf{k}') = \frac{\sqrt{2\omega'}}{2(2\pi)^{3/2}} \int \left(\varphi(\mathbf{x},0) - \frac{i}{\omega'}\pi(\mathbf{x},0)\right) e^{i\mathbf{k}'\cdot\mathbf{x}} d^3x$$
(16)

The difference of the same combination and replacing $\mathbf{k}' \to -\mathbf{k}'$ gives the adjoint mode amplitudes,

$$a^{\dagger}\left(\mathbf{k}'\right) = \frac{\sqrt{2\omega'}}{2\left(2\pi\right)^{3/2}} \int \left(\varphi\left(\mathbf{x},0\right) + \frac{i}{\omega'}\pi\left(\mathbf{x},0\right)\right) e^{-i\mathbf{k}'\cdot\mathbf{x}} d^{3}x$$
(17)

This gives the amplitudes in terms of the field and its conjugate momentum. So far, this result is classical.

Now we quantize the amplitudes by replacing φ and π by the operators, $\hat{\varphi}$ and $\hat{\pi}$. Clearly, once φ and π become operators, the amplitudes must too; there is no other field present that could become an operator instead. Dropping the primes,

$$\hat{a}(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}} \int \left(\hat{\varphi}(\mathbf{x},0) - \frac{i}{\omega'}\hat{\pi}(\mathbf{x},0)\right) e^{i\mathbf{k}\cdot\mathbf{x}} d^3x$$
(18)

$$\hat{a}^{\dagger}(\mathbf{k}) = \frac{\sqrt{2\omega}}{2(2\pi)^{3/2}} \int \left(\hat{\varphi}(\mathbf{x},0) + \frac{i}{\omega'}\hat{\pi}(\mathbf{x},0)\right) e^{-i\mathbf{k}\cdot\mathbf{x}} d^3x$$
(19)

From the commutation relations for φ and π we can compute those for a and a^{\dagger} .

$$\begin{split} \left[\hat{a} \left(\mathbf{k} \right), \hat{a}^{\dagger} \left(\mathbf{k}' \right) \right] &= \frac{\sqrt{\omega\omega'}}{2 \left(2\pi \right)^3} \int \int e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{x}'} d^3x \ d^3x' \left[\hat{\varphi} \left(\mathbf{x}, 0 \right) - \frac{i}{\omega} \hat{\pi} \left(\mathbf{x}, 0 \right), \hat{\varphi} \left(\mathbf{x}', 0 \right) + \frac{i}{\omega'} \hat{\pi} \left(\mathbf{x}', 0 \right) \right] \\ &= \frac{\sqrt{\omega\omega'}}{2 \left(2\pi \right)^3} \int \int e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{x}'} d^3x \ d^3x' \left(\frac{i}{\omega'} \left[\hat{\varphi} \left(\mathbf{x}, 0 \right), \hat{\pi} \left(\mathbf{x}', 0 \right) \right] - \frac{i}{\omega} \left[\hat{\pi} \left(\mathbf{x}, 0 \right), \hat{\varphi} \left(\mathbf{x}', 0 \right) \right] \right) \\ &= \frac{\sqrt{\omega\omega'}}{2 \left(2\pi \right)^3} \int \int e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{x}'} d^3x \ d^3x' \left(\frac{2}{\omega'} \delta^3 \left(\mathbf{x} - \mathbf{x}' \right) \right) \end{split}$$

The Dirac delta function allows us to evaluate the integrals,

$$\begin{aligned} \left[\hat{a}\left(\mathbf{k}\right), \hat{a}^{\dagger}\left(\mathbf{k}'\right)\right] &= \sqrt{\frac{\omega}{\omega'}} \frac{1}{\left(2\pi\right)^{3}} \int \int e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{x}'} d^{3}x \ d^{3}x' \delta^{3}\left(\mathbf{x}-\mathbf{x}'\right) \\ &= \sqrt{\frac{\omega}{\omega'}} \frac{1}{\left(2\pi\right)^{3}} \int e^{i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{x}} d^{3}x \\ &= \delta^{3}\left(\mathbf{k}-\mathbf{k}'\right) \end{aligned}$$

Notice that the delta function makes $\omega = \omega'$.

Exercise: Show that $[\hat{a}(\mathbf{k}), \hat{a}(\mathbf{k}')] = 0.$

Exercise: Show that $\left[\hat{a}^{\dagger}(\mathbf{k}), \hat{a}^{\dagger}(\mathbf{k}')\right] = 0.$

Finally, we summarize by the field and momentum density operators in terms of the mode amplitude operators:

$$\hat{\varphi}(\mathbf{x},t) = \frac{1}{\left(2\pi\right)^{3/2}} \int \frac{d^3k}{\sqrt{2\omega}} \left(\hat{a}\left(\mathbf{k}\right)e^{i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)} + \hat{a}^{\dagger}\left(\mathbf{k}\right)e^{-i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)}\right)$$
(20)

$$\hat{\pi}(\mathbf{x},t) = \frac{i}{\left(2\pi\right)^{3/2}} \int d^3k \sqrt{\frac{\omega}{2}} \left(\hat{a}\left(\mathbf{k}\right) e^{i\left(\omega t - \mathbf{k} \cdot \mathbf{x}\right)} - \hat{a}^{\dagger}\left(\mathbf{k}\right) e^{-i\left(\omega t - \mathbf{k} \cdot \mathbf{x}\right)}\right)$$
(21)

Next, we turn to a study of states. To begin, we require the Hamiltonian operator, which requires a bit of calculation.

1.5 Calculation of the Hamiltonian operator

This is our first typical quantum field theory calculation. They're a bit tricky to keep track of, but not really that hard. Our goal is to compute the expression for the Hamiltonian operator

$$\hat{H} \equiv \frac{\hbar}{2} \int \left(\hat{\pi}^2 + \nabla \hat{\varphi} \cdot \nabla \hat{\varphi} + m^2 \hat{\varphi}^2 \right) d^3x$$
(22)

in terms of the mode operators. Because the techniques involved are used frequently in field theory calculations, we include all the gory details.

Let's consider one term at a time. For the first,

$$\begin{split} I_{\pi} &= \frac{\hbar}{2} \int \hat{\pi}^2 d^3 x \\ &= \frac{\hbar}{2} \int d^3 x \left[\frac{i}{(2\pi)^{3/2}} \int d^3 k \sqrt{\frac{\omega}{2}} \left(\hat{a} \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right) \right. \\ &\quad \times \frac{i}{(2\pi)^{3/2}} \int d^3 k' \sqrt{\frac{\omega'}{2}} \left(\hat{a} \left(\mathbf{k}' \right) e^{i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x}\right)} - \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{-i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x}\right)} \right) \right] \\ &= -\frac{1}{4} \frac{\hbar}{(2\pi)^3} \int d^3 x \int d^3 k \int d^3 k' \sqrt{\omega \omega'} \left(\hat{a} \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i\left(\omega t - \mathbf{k} \cdot \mathbf{x}\right)} \right) \left(\hat{a} \left(\mathbf{k}' \right) e^{i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x}\right)} - \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{-i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x}\right)} \right) \\ &= -\frac{1}{4} \frac{\hbar}{(2\pi)^3} \int d^3 x \int d^3 k \int d^3 k' \sqrt{\omega \omega'} \left[\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) e^{i\left((\omega + \omega')t - \left(\mathbf{k} + \mathbf{k}'\right) \cdot \mathbf{x}\right)} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{i\left((\omega - \omega')t - \left(\mathbf{k} - \mathbf{k}'\right) \cdot \mathbf{x}\right)} \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) e^{-i\left(\left((\omega - \omega')t - \left(\mathbf{k} - \mathbf{k}'\right) \cdot \mathbf{x}\right)} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{-i\left(\left((\omega + \omega')t - \left(\mathbf{k} + \mathbf{k}'\right) \cdot \mathbf{x}\right)} \right] \end{split}$$

The integral over d^3x , produces Dirac delta functions, which we integrate immediately:

$$I_{\pi} = -\frac{\hbar}{4} \int d^{3}k \int d^{3}k' \sqrt{\omega\omega'} \left[\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} + \mathbf{k'} \right) e^{i\left(\omega + \omega'\right)t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{i\left(\omega - \omega'\right)t} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{i\left(\omega - \omega'\right)t} \\ - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} + \mathbf{k'} \right) e^{-i\left(\omega + \omega'\right)t} \right] \\ = - \frac{\hbar}{4} \int d^{3}k \, \omega \left[\hat{a} \left(\mathbf{k} \right) \hat{a} \left(- \mathbf{k} \right) e^{2i\omega t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(- \mathbf{k} \right) e^{-2i\omega t} \right]$$

We follow the same steps for the remaining two terms in the Hamiltonian. Inserting the gradient of Eq.(20), the second term becomes

$$\begin{split} I_{\nabla\varphi} &= \frac{\hbar}{2} \int \boldsymbol{\nabla} \hat{\varphi} \cdot \boldsymbol{\nabla} \hat{\varphi} d^{3}x \\ &= \frac{\hbar}{2} \frac{1}{(2\pi)^{3}} \int d^{3}x \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} \left(-i\mathbf{k} \right) \cdot \left(-i\mathbf{k'} \right) \left(\hat{a} \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right) \left(\hat{a} \left(\mathbf{k'} \right) e^{i\left(\omega' t - \mathbf{k'} \cdot \mathbf{x} \right)} - \hat{a}^{\dagger} \left(\mathbf{k'} \right) e^{-i} \\ &= -\frac{\hbar}{2} \frac{1}{(2\pi)^{3}} \int d^{3}x \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} \mathbf{k} \cdot \mathbf{k'} \left[\left(\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) e^{i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} + \mathbf{k'}\right) \cdot \mathbf{x}\right)} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) e^{i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} \right) \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) e^{-i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) e^{-i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} \right] \\ &= -\frac{\hbar}{2} \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} \mathbf{k} \cdot \mathbf{k'} \left[\left(\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} + \mathbf{k'} \right) e^{i\left(\omega + \omega'\right)t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{i\left(\omega - \omega'\right)t} \right) \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{i\left(\omega - \omega'\right)t} \right) \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} \right) \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} \right) \\ &- \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k'} \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i\left(\omega - \omega'\right)t} \right) \\ &= -\frac{\hbar}{4} \int d^{3}k \frac{\mathbf{k}^{2}}{\omega} \left[-\hat{a} \left(\mathbf{k} \right) \hat{a} \left(-\mathbf{k} \right) e^{2i\omega t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-2i\omega t} \right] \end{aligned}$$

As before, the d^3x integrals of the four terms give four Dirac delta functions and the d^3k' integrals become trivial. It is not hard to see the pattern that is emerging. The $\frac{\mathbf{k}\cdot\mathbf{k}}{\omega}$ term will combine nicely with the ω from the $\hat{\pi}^2$ integral and a corresponding m^2 term from the final integral to give a cancellation. The crucial thing is to keep track of the signs.

The third and final term is

$$\begin{split} I_{m} &= \frac{\hbar}{2} \int m^{2} \hat{\varphi}^{2} d^{3}x \\ &= \frac{\hbar}{2} \frac{1}{(2\pi)^{3}} \int d^{3}x \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} m^{2} \left(\hat{a} \left(\mathbf{k} \right) e^{i\left(\omega t - \mathbf{k} \cdot \mathbf{x} \right)} + \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i\left(\omega t - \mathbf{k} \cdot \mathbf{x} \right)} \right) \left(\hat{a} \left(\mathbf{k}' \right) e^{i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x} \right)} + \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{-i\left(\omega' t - \mathbf{k}' \cdot \mathbf{x} \right)} \right) \\ &= \frac{\hbar}{2} \frac{1}{(2\pi)^{3}} \int d^{3}x \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} m^{2} \left[\left(\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) e^{i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} + \mathbf{k}' \right) \cdot \mathbf{x} \right)} + \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k}' \right) \cdot \mathbf{x} \right)} \right) \\ &\quad + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) e^{-i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k}' \right) \cdot \mathbf{x} \right)} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) e^{-i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} - \mathbf{k}' \right) \cdot \mathbf{x} \right)} \right] \\ &= \frac{\hbar}{2} \int \frac{d^{3}k}{\sqrt{2\omega}} \int \frac{d^{3}k'}{\sqrt{2\omega'}} m^{2} \left[\left(\hat{a} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} + \mathbf{k}' \right) e^{i\left(\omega - \omega'\right)t} + \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{i\left(\omega - \omega'\right)t} \right) \\ &\quad + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{i\left(\omega - \omega'\right)t} \right) \\ &\quad + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k}' \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{-i\left(\omega - \omega'\right)t} \right) \\ &\quad + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{-i\left(\omega - \omega'\right)t} + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) \delta^{3} \left(\mathbf{k} - \mathbf{k}' \right) e^{-i\left(\omega - \omega'\right)t} \right) \\ &\quad + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{$$

Now we can combine all three terms:

$$\begin{split} \hat{H} &\equiv \frac{\hbar}{2} \int \left(\hat{\pi}^2 + \boldsymbol{\nabla} \hat{\varphi} \cdot \boldsymbol{\nabla} \hat{\varphi} + m^2 \hat{\varphi}^2 \right) d^3x \\ &= I_{\pi} + I_{\nabla \varphi} + I_m \\ &= -\frac{\hbar}{4} \int d^3k \, \omega \left[\hat{a} \left(\mathbf{k} \right) \hat{a} \left(-\mathbf{k} \right) e^{2i\omega t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(-\mathbf{k} \right) e^{-2i\omega t} \right] \\ &- \frac{\hbar}{4} \int d^3k \, \frac{\mathbf{k}^2}{\omega} \left[-\hat{a} \left(\mathbf{k} \right) \hat{a} \left(-\mathbf{k} \right) e^{2i\omega t} - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(-\mathbf{k} \right) e^{-2i\omega t} \right] \\ &+ \frac{\hbar}{4} \int d^3k \, \frac{m^2}{\omega} \left[\hat{a} \left(\mathbf{k} \right) \hat{a} \left(-\mathbf{k} \right) e^{2i\omega t} + \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(-\mathbf{k} \right) e^{-2i\omega t} \right] \end{split}$$

$$= -\frac{\hbar}{4} \int d^3k \left(\omega - \frac{\mathbf{k}^2}{\omega} - \frac{m^2}{\omega}\right) \hat{a}\left(\mathbf{k}\right) \hat{a}\left(-\mathbf{k}\right) e^{2i\omega t} - \frac{\hbar}{4} \int d^3k \left(-\omega - \frac{\mathbf{k}^2}{\omega} - \frac{m^2}{\omega}\right) \hat{a}\left(\mathbf{k}\right) \hat{a}^{\dagger}\left(\mathbf{k}\right) \\ -\frac{\hbar}{4} \int d^3k \left(-\omega - \frac{\mathbf{k}^2}{\omega} - \frac{m^2}{\omega}\right) \hat{a}^{\dagger}\left(\mathbf{k}\right) \hat{a}\left(\mathbf{k}\right) - \frac{\hbar}{4} \int d^3k \left(\omega - \frac{\mathbf{k}^2}{\omega} - \frac{m^2}{\omega}\right) \hat{a}^{\dagger}\left(\mathbf{k}\right) \hat{a}^{\dagger}\left(-\mathbf{k}\right) e^{-2i\omega t}$$

Since

$$\omega^2 - \mathbf{k}^2 = m^2$$

the Hamiltonian becomes

$$\hat{H} = -\frac{\hbar}{4} \int d^3k \, (-2\omega) \,\hat{a} \left(\mathbf{k}\right) \hat{a}^{\dagger} \left(\mathbf{k}\right) - \frac{\hbar}{4} \int d^3k \, (-2\omega) \,\hat{a}^{\dagger} \left(\mathbf{k}\right) \hat{a} \left(\mathbf{k}\right)$$
$$= \frac{1}{2} \int d^3k \, \hbar\omega \left(\hat{a} \left(\mathbf{k}\right) \hat{a}^{\dagger} \left(\mathbf{k}\right) + \hat{a}^{\dagger} \left(\mathbf{k}\right) \hat{a} \left(\mathbf{k}\right)\right)$$

If we commute $\hat{a}(\mathbf{k})$ and $\hat{a}^{\dagger}(\mathbf{k})$ in the first term on the right, we encounter a problem:

$$\hat{H} = \frac{1}{2} \int d^3k \, \hbar\omega \left(\hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \delta^3 \left(\mathbf{k} - \mathbf{k} \right) \right)$$
$$= \int d^3k \, \hbar\omega \left(\hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \frac{1}{2} \delta^3 \left(\mathbf{k} - \mathbf{k} \right) \right)$$

This is very close to a sensible result, but the constant term is problematic.

1.6 Our first infinity

The form of the Hamiltonian found above displays an obvious problem – the final term,

$$\frac{1}{2}\int d^{3}k\,\hbar\omega\delta^{3}\left(0\right)$$

diverges in several ways. Most obviously, the triple Dirac delta function is evaluated at 0 and therefore diverges. Even if it were not present, the remaining integral, $\int d^3k \omega$, itself diverges.

While the constant "ground state energy" of the harmonic oscillator, $\frac{1}{2}\hbar\omega$, causes no probem in quantum mechanics, the presence of such an energy term for each mode of quantum field theory leads to an infinite energy for the vacuum state. Fortunately, a simple trick allows us to eliminate this divergence throughout our calculations. To see how it works, notice that anytime we have a product of two or more fields at the same point, we develop some terms of the general form

$$\hat{\varphi}(\mathbf{x}) \hat{\varphi}(\mathbf{x}) \sim \hat{a}(\omega, \mathbf{k}) \hat{a}^{\dagger}(\omega, \mathbf{k}) + \dots$$

which have $\hat{a}^{\dagger}(\omega, \mathbf{k})$ to the right of $\hat{a}(\omega, \mathbf{k})$. When such products act on the vacuum state, the $\hat{a}^{\dagger}(\omega, \mathbf{k})$ gives a nonvanishing contribution, and if we sum over all wave vectors we get a divergence. The solution is simply to impose a rule that changes the order of the creation and annihilation operators. This is called *normal ordering*, and is denoted by enclosing the product in colons. Thus, we define

$$\hat{a}(\omega, \mathbf{k}) \hat{a}^{\dagger}(\omega, \mathbf{k}) :\equiv \hat{a}^{\dagger}(\omega, \mathbf{k}) \hat{a}(\omega, \mathbf{k})$$

and more generally, normal ordering requires us to place all creation operators to the left of anihilation operators. There is always an ordering ambituity when building functions of $\hat{\varphi}$ and $\hat{\pi}$, since these do not commute. We resolve the ordering ambiguity by writing the function in terms of $\hat{a}(\omega, \mathbf{k})$ and $\hat{a}^{\dagger}(\omega, \mathbf{k})$ and normal ordering,

$$f(\varphi, \pi) \Rightarrow : f(\hat{\varphi}, \hat{\pi}):$$

Applied to the Hamiltonian, we define

$$\hat{H} = \frac{\hbar}{2} \int : \left(\hat{\pi}^2 + \boldsymbol{\nabla} \hat{\varphi} \cdot \boldsymbol{\nabla} \hat{\varphi} + m^2 \hat{\varphi}^2 \right) : d^3x$$

$$= \frac{1}{2} \int d^3k \, \hbar \omega : \left(\hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) + \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) \right) :$$

and this results in

$$\hat{H} = \int d^3k \,\hbar\omega \hat{a}^{\dagger}\left(\mathbf{k}\right) \hat{a}\left(\mathbf{k}\right)$$
(23)

This expression gives zero for the vacuum state, and is finite for all states with a finite number of particles. While this procedure may seem a bit ad hoc, recall that the ordering of operators in any quantum expression is one thing that cannot be determined from the classical framework using canonical quantization. It is therefore reasonable to use whatever ordering convention gives the most sensible results.

1.7 States of the Klein-Gordon field

The similarity between the field Hamiltonian and the harmonic oscillator makes it easy to interpret this result. We begin the observation that the expectation values of \hat{H} are bounded below. This follows because for any normalized state $|\alpha\rangle$ we have

$$\begin{aligned} \langle \alpha | \hat{H} | \alpha \rangle &= \langle \alpha | \int d^3 k \, \hbar \omega \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) | \alpha \rangle \\ &= \int d^3 k \, \hbar \omega \left(\langle \alpha | \, \hat{a}^{\dagger} \left(\mathbf{k} \right) \right) \left(\hat{a} \left(\mathbf{k} \right) | \alpha \rangle) \end{aligned}$$

This is positive definite, since if we let $|\beta\rangle = \hat{a}(\mathbf{k}) |\alpha\rangle$, then $\langle\beta| = \langle\alpha| \hat{a}^{\dagger}(\mathbf{k})$, so

$$\begin{aligned} \langle \alpha | \hat{H} | \alpha \rangle &= \int d^3k \, \hbar \omega \, \langle \alpha | \, \hat{a}^{\dagger}(\mathbf{k}) \hat{a}(\mathbf{k}) \, | \alpha \rangle \\ &= \int d^3k \, \hbar \omega \, \langle \beta | \beta \rangle \\ &> 0 \end{aligned}$$

since the integrand is positive definite. However, we can show that the action of $\hat{a}(\mathbf{k})$ lowers the eigenvalues of \hat{H} . Consider the commutator of $\hat{a}(\mathbf{k})$ with the Hamiltonian,

$$\begin{split} \left[\hat{H}, \hat{a} \left(\mathbf{k} \right) \right] &= \left[\int d^3 k' \hbar \omega' \hat{a}^{\dagger} \left(\mathbf{k}' \right) \hat{a} \left(\mathbf{k}' \right), \hat{a} \left(\mathbf{k} \right) \right] \\ &= \int d^3 k' \hbar \omega' \left[\hat{a}^{\dagger} \left(\mathbf{k}' \right), \hat{a} \left(\mathbf{k} \right) \right] \hat{a} \left(\mathbf{k}' \right) \\ &= -\int d^3 k' \hbar \omega' \delta^3 \left(\mathbf{k} - \mathbf{k}' \right) \hat{a} \left(\mathbf{k}' \right) \\ &= -\hbar \omega \, \hat{a} \left(\mathbf{k} \right) \end{split}$$

Therefore, if $|\alpha\rangle$ is an eigenstate of \hat{H} with $\hat{H} |\alpha\rangle = \alpha |\alpha\rangle$ then so is $\hat{a}(\mathbf{k}) |\alpha\rangle$ because

$$\hat{H}(\hat{a}(\mathbf{k})|\alpha\rangle) = \left[\hat{H}, \hat{a}(\mathbf{k})\right]|\alpha\rangle + \hat{a}(\mathbf{k})\hat{H}|\alpha\rangle$$
$$= -\hbar\omega\hat{a}(\mathbf{k})|\alpha\rangle + \hat{a}(\mathbf{k})\alpha|\alpha\rangle$$
$$= (\alpha - \hbar\omega)(\hat{a}(\mathbf{k})|\alpha\rangle)$$

Moreover, the eigenvalue of the new eigenstate is *lower* than α . Since the eigenvalues are bounded below, there must exist a state such that

$$\hat{a}\left(\mathbf{k}\right)\left|0\right\rangle = 0\tag{24}$$

for all values of **k**. The state $|0\rangle$ is called the *vacuum state* and the operators $\hat{a}(\mathbf{k})$ are called annihilation operators. From the vacuum state, we can construct the entire spectrum of eigenstates of the Hamiltonian. First, notice that the vacuum state is a minimal eigenstate of \hat{H} :

$$\hat{H} |0\rangle = \int d^{3}k' \hbar \omega' \hat{a}^{\dagger} (\mathbf{k}') \hat{a} (\mathbf{k}') |0\rangle$$

= 0

Now, we act on the vacuum state with $\hat{a}^{\dagger}(\mathbf{k})$ to produce new eigenstates.

Exercise: Prove that $|\mathbf{k}\rangle = \hat{a}^{\dagger}(\mathbf{k}) |0\rangle$ is an eigenstate of \hat{H} with energy eigenvalue $\hbar\omega$.

We can build infinitely many states in two ways. First, just like the harmonic oscillator states, we can apply the creation operator $\hat{a}^{\dagger}(\mathbf{k})$ as many times as we like. Such a state contains multiple particles with energy $\hbar\omega$. Second, we can apply creation operators of different \mathbf{k} :

$$|\mathbf{k}',\mathbf{k}\rangle = \hat{a}^{\dagger}(\mathbf{k}')\hat{a}^{\dagger}(\mathbf{k})|0\rangle = \hat{a}^{\dagger}(\mathbf{k})\hat{a}^{\dagger}(\mathbf{k}')|0\rangle$$

This state contains two particles, one with energy $\hbar\omega$ and the other with energy $\hbar\omega'$.

As with the harmonic oscillator, we can introduce a number operator to measure the number of quanta in a given state. The number operator is just the sum over all modes of the number operator for a given mode:

$$\hat{N} = \int : \left(\hat{a}^{\dagger}(\mathbf{k}) \hat{a}(\mathbf{k}) \right) : d^{3}k$$

$$= \int \hat{a}^{\dagger}(\mathbf{k}) \hat{a}(\mathbf{k}) d^{3}k$$

Exercise: By applying \hat{N} , compute the number of particles in the state

$$|\mathbf{k}',\mathbf{k}\rangle = \hat{a}^{\dagger}(\mathbf{k}')\hat{a}^{\dagger}(\mathbf{k})|0\rangle$$

Notice that creation and annihilation operators for different modes all commute with one another, e.g.,

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

when $\mathbf{k}' \neq \mathbf{k}$.

1.8 Poincaré transformations of Klein-Gordon fields

Now let's examine the Lorentz transformation and translation properties of scalar fields. For this we need to construct quantum operators which generate the required transformations. Since the translations are the simplest, we begin with them.

We have observed that the spacetime translation generators forming a basis for the Lie algebra of translations (and part of the basis of the Poincaré Lie algebra) resemble the energy and momentum operators of quantum mechanics. Moreover, Noether's theorem tells us that energy and momentum are conserved as a result of translation symmetry of the action. We now need to bring these insights into the realm of quantum fields. From our discussion in Chapter 1, using the Klein-Gordon Lagrangian density from eq.(2), we have the conserved stress-energy tensor,

$$T^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu}\phi)} \partial^{\nu}\phi - \mathcal{L}\eta^{\mu\nu}$$
$$= \partial^{\mu}\varphi \partial^{\nu}\varphi - \frac{1}{2}\eta^{\mu\nu} \left(\pi^{2} - \nabla\varphi \cdot \nabla\varphi - m^{2}\varphi^{2}\right)$$

which leads to the conserved charges,

$$P^{\mu} = \int T^{\mu 0} d^3 x$$

and the natural extension of this observation is to simply replace the products of fields in $T^{\mu 0}$ with normalordered field operators. We therefore write

$$\hat{P}^{\mu} \equiv \int :\hat{T}^{\mu 0}: d^3x$$

First, for the time component,

$$\begin{split} \hat{P}^0 &= \int :\hat{T}^{00}: d^3x \\ &= \int :\partial^0 \hat{\varphi} \partial^0 \hat{\varphi} - \frac{1}{2} \eta^{00} \left(\hat{\pi}^2 - \nabla \hat{\varphi} \cdot \hat{\varphi} - m^2 \hat{\varphi}^2 \right): d^3x \\ &= \frac{1}{2} \int :\hat{\pi}^2 + \nabla \hat{\varphi} \cdot \nabla \hat{\varphi} + m^2 \hat{\varphi}^2: d^3x \\ &= \hat{H} \end{split}$$

This is promising!

Now consider the momentum operators:

$$\begin{split} \hat{P}^{i} &\equiv \int :\hat{T}^{i0}:d^{3}x \\ &= \int :\partial^{i}\hat{\varphi}\partial^{0}\hat{\varphi} - \frac{1}{2}\eta^{i0}\left(\hat{\pi}^{2} - \nabla\hat{\varphi}\cdot\hat{\varphi} - m^{2}\hat{\varphi}^{2}\right):d^{3}x \\ &= \int :\partial^{i}\hat{\varphi}\,\hat{\pi}:d^{3}x \\ \hat{\mathbf{P}} &= \int :\boldsymbol{\nabla}\hat{\varphi}\,\hat{\pi}:d^{3}x \end{split}$$

Exercise: By substituting the field operators, eq.(20) and eq.(21), into the integral for \hat{P}^i , show that

$$\hat{\mathbf{P}} = \frac{1}{2} \int \hbar \mathbf{k} \left[-\hat{a}(\mathbf{k})\hat{a}(-\mathbf{k})e^{2i\omega t} + \hat{a}(\mathbf{k})\hat{a}^{\dagger}(\mathbf{k}) + \hat{a}^{\dagger}(\mathbf{k})\hat{a}(\mathbf{k}) - \hat{a}^{\dagger}(\mathbf{k})\hat{a}^{\dagger}(-\mathbf{k})e^{-2i\omega t} \right] d^{3}k$$

The calculation is similar to the computation of the Hamiltonian operator above, except there is only one term to consider.

We can simplify this result for $\hat{\mathbf{P}}$ using a parity argument. Consider the effect of parity on the first integral. Since the volume form together with the limits is invariant under $\mathbf{k} \to -\mathbf{k}$,

$$\iiint_{-\infty}^{\infty} d^3k \quad \to \quad \iiint_{\infty}^{-\infty} (-1)^3 d^3k = \iiint_{-\infty}^{\infty} d^3k$$

and $\omega\left(-\mathbf{k}\right) = \omega\left(\mathbf{k}\right)$, the first integral satisfies

$$\begin{aligned} \hat{\mathbf{I}}_1 &= \frac{1}{2} \int d^3k \ \hbar \mathbf{k} \ \hat{a}(\mathbf{k}) \hat{a}(-\mathbf{k}) e^{2i\omega t} \\ &= \frac{1}{2} \int d^3k \ (-\hbar \mathbf{k}) \ \hat{a}(-\mathbf{k}) \hat{a}(\mathbf{k}) e^{2i\omega t} \\ &= -\frac{1}{2} \int d^3k \ \hbar \mathbf{k} \ \hat{a}(\mathbf{k}) \hat{a}(-\mathbf{k}) e^{2i\omega t} \\ &= -\hat{\mathbf{I}}_1 \end{aligned}$$

and therefore $\hat{\mathbf{I}}_1 = 0$. The final term vanishes in the same way, so the momentum operator reduces to

$$\begin{aligned} \hat{\mathbf{P}} &= \int :\partial^i \hat{\varphi} \ \hat{\pi} : d^3 x \\ &= \frac{1}{2} \int \hbar \mathbf{k} : \left(\hat{a}(\mathbf{k}) \hat{a}^{\dagger}(\mathbf{k}) + \hat{a}^{\dagger}(\mathbf{k}) \hat{a}(\mathbf{k}) \right) : d^3 k \\ &= \int \hbar \mathbf{k} \ \hat{a}(\mathbf{k}) \hat{a}^{\dagger}(\mathbf{k}) d^3 k \end{aligned}$$

Once again, this makes sense; moreover, they are suitable for translation generators since they all commute.

In a similar way, we can compute the operators $\hat{M}^{\alpha\beta}$, and show that the commutation relations of the full set reproduce the Poincaré Lie algebra,

$$\begin{bmatrix} \hat{M}^{\alpha\beta}, \hat{M}^{\mu\nu} \end{bmatrix} = \eta^{\beta\mu} \hat{M}^{\alpha\nu} - \eta^{\beta\nu} \hat{M}^{\alpha\mu} - \eta^{\alpha\mu} \hat{M}^{\beta\nu} - \eta^{\alpha\nu} \hat{M}^{\beta\mu} \\ \begin{bmatrix} \hat{M}^{\alpha\beta}, \hat{P}^{\mu} \end{bmatrix} = \eta^{\mu\alpha} \hat{P}^{\beta} - \eta^{\mu\beta} \hat{P}^{\alpha} \\ \begin{bmatrix} \hat{P}^{\alpha}, \hat{P}^{\beta} \end{bmatrix} = 0$$

The notable accomplishment here is that we have shown that even after quantization, the symmetry algebra not only survives, but can be built from the quantum field operators. This is far from obvious, because the commutation relations for the field operators are simply imposed by the rules of canonical quantization and have nothing to do, a priori, with the commutators of the symmetry algebra. One consequence, as noted above, is that the Casimir operators of the Poincaré algebra may be used to label *quantum* states.

2 Quantization of the complex scalar field

2.1 Classical Hamiltonian formulation

The complex scalar field provides a slight generalization of the real scalar field. As before we begin with the Lagrangian, Eq.(??)

$$L = \int \left(\partial^{\alpha}\varphi^*\partial_{\alpha}\varphi - m^2\varphi^*\varphi\right)d^3x \tag{25}$$

This has twice the degrees of freedom as the real Klein-Gordon field, and introduces an extra symmetry. While we could realize the two degrees of freedom by expanding $\varphi = \varphi_R + i\varphi_I$, treating φ and φ^* as the independent variables yields the same results.

We define the conjugate momentum densities to each of φ and φ^* as the functional derivatives L with respect to φ and φ^* :

$$\pi \equiv \frac{\delta L}{\delta\left(\partial_0\varphi\right)} = \partial^0\varphi^*\left(\mathbf{x}\right) \tag{26}$$

and similarly

$$\pi^* \equiv \frac{\delta L}{\delta\left(\partial_0 \varphi^*\right)} = \partial^0 \varphi\left(\mathbf{x}\right) \tag{27}$$

The action and Lagrangian density, written in terms of these momenta, are therefore

$$S = \int (\pi \pi^* - \nabla \varphi^* \cdot \nabla \varphi - m^2 \varphi^* \varphi) d^4 x$$

$$\mathcal{L} = \pi \pi^* - \nabla \varphi^* \cdot \nabla \varphi - m^2 \varphi^* \varphi$$

The Hamiltonian is defined as

$$H \equiv \int (\pi \partial_0 \varphi + \pi^* \partial_0 \varphi^*) d^3 x - L$$

=
$$\int (\pi \pi^* + \pi^* \pi) - (\pi \pi^* - \nabla \varphi^* \cdot \nabla \varphi - m^2 \varphi^* \varphi) d^3 x$$

and therefore

$$H = \int \left(\pi^* \pi + \nabla \varphi^* \cdot \nabla \varphi + m^2 \varphi^* \varphi\right) d^3 x$$
(28)

Hamilton's equations are:

$$\begin{split} \dot{\varphi} \left(\mathbf{x} \right) &= \frac{\delta H}{\delta \pi \left(\mathbf{x} \right)} \\ \dot{\pi} \left(\mathbf{x} \right) &= -\frac{\delta H}{\delta \varphi \left(\mathbf{x} \right)} \\ \dot{\varphi}^{*} \left(\mathbf{x} \right) &= \frac{\delta H}{\delta \pi^{*} \left(\mathbf{x} \right)} \\ \dot{\pi}^{*} \left(\mathbf{x} \right) &= -\frac{\delta H}{\delta \varphi^{*} \left(\mathbf{x} \right)} \end{split}$$

Exercise: Prove that Hamilton's equations reproduce the field equations for φ and φ^* .

Now write the field equations in terms of functional Poisson brackets which – remembering to sum the derivatives over all independent fields – are given for functionals $f = f[\varphi, \pi, \varphi^*, \pi^*]$ and $g = g[\varphi, \pi, \varphi^*, \pi^*]$ by

$$\{f,g\} \equiv \int d^3x \left(\frac{\delta f}{\delta \pi(\mathbf{x})} \frac{\delta g}{\delta \varphi(\mathbf{x})} + \frac{\delta f}{\delta \pi^*(\mathbf{x})} \frac{\delta g}{\delta \varphi^*(\mathbf{x})} - \frac{\delta f}{\delta \varphi(\mathbf{x})} \frac{\delta g}{\delta \pi(\mathbf{x})} - \frac{\delta f}{\delta \varphi^*(\mathbf{x})} \frac{\delta g}{\delta \pi^*(\mathbf{x})}\right)$$
(29)

The result is the just what we would guess from the real case,

$$\begin{aligned} \left\{ \pi \left(\mathbf{x} \right), \varphi \left(\mathbf{y} \right) \right\} &= \int \left(\frac{\delta \pi \left(\mathbf{x} \right)}{\delta \pi \left(\mathbf{x}' \right)} \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \varphi \left(\mathbf{x}' \right)} + 0 - \frac{\delta \pi \left(\mathbf{x} \right)}{\delta \varphi \left(\mathbf{x}' \right)} \frac{\delta \varphi \left(\mathbf{y} \right)}{\delta \pi \left(\mathbf{x}' \right)} - 0 \right) d^3 x \\ &= \int \delta^3 \left(\mathbf{x} - \mathbf{x}' \right) \delta^3 \left(\mathbf{y} - \mathbf{x} \right) d^3 x \\ &= \delta^3 \left(\mathbf{x} - \mathbf{y} \right) \\ \left\{ \pi^* \left(\mathbf{x} \right), \varphi^* \left(\mathbf{y} \right) \right\} &= \delta^3 (\mathbf{x} - \mathbf{y}) \end{aligned}$$

with all other brackets vanishing.

Exercise: Check that Hamilton's equations

$$\begin{aligned} \dot{\varphi}(\mathbf{x}) &= \{H\left(\varphi, \pi, \varphi^*, \pi^*\right), \varphi(\mathbf{x}')\} \\ \dot{\varphi}^*(\mathbf{x}) &= \{H\left(\varphi, \pi, \varphi^*, \pi^*\right), \varphi^*(\mathbf{x}')\} \\ \dot{\pi}(\mathbf{x}) &= \{H\left(\varphi, \pi, \varphi^*, \pi^*\right), \pi(\mathbf{x}')\} \\ \dot{\pi}^*(\mathbf{x}) &= \{H\left(\varphi, \pi, \varphi^*, \pi^*\right), \pi^*(\mathbf{x}')\} \end{aligned}$$

reproduce Hamilton's equations.

Now we quantize, replacing fields by operators and Poisson brackets by equal-time commutators:

$$\left[\hat{\pi}\left(\mathbf{x},t\right),\hat{\varphi}\left(\mathbf{y},t\right)\right] = i\hbar\delta^{3}\left(\mathbf{x}-\mathbf{y}\right)$$
(30)

$$\left[\hat{\pi}^{*}\left(\mathbf{x},t\right),\hat{\varphi}^{*}\left(\mathbf{y},t\right)\right] = i\hbar\delta^{3}\left(\mathbf{x}-\mathbf{y}\right)$$
(31)

with all other pairs commuting. Now we seek free field solutions satisfying these quantization relations.

2.2 Mode amplitudes of the complex scalar field

The solution proceeds as before, by starting with solutions for the classical theory. The field equations

$$\Box \varphi = -\frac{m^2}{\hbar^2} \varphi$$
$$\Box \varphi^* = -\frac{m^2}{\hbar^2} \varphi^*$$

are complex conjugates of each other. The only difference from the real case is that we no longer restrict to real plane waves. This leaves the amplitudes independent:

$$\varphi(\mathbf{x},t) = Ae^{\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{x})} + B^{\dagger}e^{-\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{x})}$$
(32)

Substituting into the field equation we have

$$\Box \varphi = \left(\frac{i}{\hbar}\right)^2 p_{\alpha} p^{\alpha} A e^{\frac{i}{\hbar}(Et - \mathbf{p} \cdot \mathbf{x})} + \left(-\frac{i}{\hbar}\right)^2 p_{\alpha} p^{\alpha} B^{\dagger} e^{-\frac{i}{\hbar}(Et - \mathbf{p} \cdot \mathbf{x})}$$
$$= -\frac{1}{\hbar^2} p_{\alpha} p^{\alpha} \varphi(\mathbf{x}, t)$$

so again we require the energy condition

$$p_{\alpha}p^{\alpha} = m^2$$

We can solve this for the energy,

$$E_+ = \sqrt{\mathbf{p}^2 + m^2}$$
$$E_- = -\sqrt{\mathbf{p}^2 + m^2}$$

The general Fourier superposition is

$$\begin{aligned} \varphi\left(\mathbf{x},t\right) &= \frac{1}{\left(2\pi\right)^{3/2}} \int \sqrt{2E} \left(a\left(E,\mathbf{p}\right)e^{\frac{i}{\hbar}\left(p_{\alpha}x^{\alpha}\right)} + b^{\dagger}\left(E,\mathbf{p}\right)e^{-\frac{i}{\hbar}\left(p_{\alpha}x^{\alpha}\right)}\right) \delta\left(p_{\alpha}p^{\alpha} - m^{2}\right)\Theta(E)\hbar^{-4}d^{4}p \\ &= \frac{1}{\left(2\pi\right)^{3/2}} \int \frac{d^{3}k}{\sqrt{2\omega}} \left(a\left(\mathbf{k}\right)e^{i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)} + b^{\dagger}\left(\mathbf{k}\right)e^{-i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)}\right) \end{aligned}$$

Collecting this together with the the conjugate field and the momenta,

$$\varphi(\mathbf{x},t) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k}{\sqrt{2\omega}} \left(a\left(\mathbf{k}\right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} + b^{\dagger}\left(\mathbf{k}\right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right)$$
(33)

$$\varphi^*(\mathbf{x},t) = \frac{1}{\left(2\pi\right)^{3/2}} \int \frac{d^3k}{\sqrt{2\omega}} \left(b\left(\mathbf{k}\right)e^{i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)} + a^{\dagger}\left(\mathbf{k}\right)e^{-i\left(\omega t - \mathbf{k}\cdot\mathbf{x}\right)}\right)$$
(34)

$$\pi(\mathbf{x},t) = \frac{i}{(2\pi)^{3/2}} \int \sqrt{\frac{\omega}{2}} d^3k \left(b(\mathbf{k}) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - a^{\dagger}(\mathbf{k}) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right)$$
(35)

$$\pi^* \left(\mathbf{x}, t \right) = \frac{i}{\left(2\pi\right)^{3/2}} \int \sqrt{\frac{\omega}{2}} d^3k \left(a\left(\mathbf{k} \right) e^{i\left(\omega t - \mathbf{k} \cdot \mathbf{x} \right)} - b^{\dagger}\left(\mathbf{k} \right) e^{-i\left(\omega t - \mathbf{k} \cdot \mathbf{x} \right)} \right)$$
(36)

Notice that we may obtain the conjugate expressions, Eqs.(34) and (36) simply by interchanging a with b, and interchanging a^{\dagger} with b^{\dagger} .

We need to invert these Fourier integrals to solve for $a(\mathbf{k}), b(\mathbf{k}), a^{\dagger}(\mathbf{k})$ and $b^{\dagger}(\mathbf{k})$.

Exercise: By taking inverse Fourier integrals, show that

$$a(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{\omega}{2}} \int d^3x \left(\varphi(\mathbf{x}, 0) - \frac{i}{\omega} \pi^*(\mathbf{x}, 0)\right) e^{i\mathbf{k}\cdot\mathbf{x}}$$
(37)

$$b(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \sqrt{\frac{\omega}{2}} \int d^3x \left(\varphi^*(\mathbf{x}, 0) - \frac{i}{\omega}\pi(\mathbf{x}, 0)\right) e^{i\mathbf{k}\cdot\mathbf{x}}$$
(38)

It follows immediately from this exercise that the conjugate mode amplitudes are given by

$$a^{*}\left(\mathbf{k}\right) = \frac{1}{\left(2\pi\right)^{3/2}} \sqrt{\frac{\omega}{2}} \int d^{3}x \left(\varphi^{*}\left(\mathbf{x},0\right) + \frac{i}{\omega}\pi\left(\mathbf{x},0\right)\right) e^{-i\mathbf{k}\cdot\mathbf{x}}$$
(39)

$$b^{*}(\mathbf{k}) = \frac{1}{\left(2\pi\right)^{3/2}} \sqrt{\frac{\omega}{2}} \int d^{3}x \left(\varphi\left(\mathbf{x},0\right) + \frac{i}{\omega}\pi^{*}\left(\mathbf{x},0\right)\right) e^{-i\mathbf{k}\cdot\mathbf{x}}$$
(40)

2.3 Quantization

We can now move to study the quantum operators. When the fields become operators the complex conjugates above become adjoints (for example, $a^*(\mathbf{k}) \to a^{\dagger}(\mathbf{k})$). We next find the commutation relations that hold among the four operators $\hat{a}(\mathbf{k}), \hat{b}(\mathbf{k}), \hat{a}^{\dagger}(\mathbf{k})$ and $\hat{b}^{\dagger}(\mathbf{k})$.

Exercise: From the commutation relations for the fields and conjugate momenta, Eqs.(30) and (31), show that

$$\begin{bmatrix} \hat{a} (\mathbf{k}), \hat{a}^{\dagger} (\mathbf{k}') \end{bmatrix} = \delta^{3} (\mathbf{k} - \mathbf{k}')$$
$$\begin{bmatrix} \hat{b} (\mathbf{k}), \hat{b}^{\dagger} (\mathbf{k}') \end{bmatrix} = \delta^{3} (\mathbf{k} - \mathbf{k}')$$

Exercise: From the commutation relations for the fields and conjugate momenta, eqs.(30) and (31), show that

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$$\begin{bmatrix} \hat{a} (\mathbf{k}), \hat{b} (\mathbf{k}') \end{bmatrix} = 0$$
$$\begin{bmatrix} \hat{a} (\mathbf{k}), \hat{b}^{\dagger} (\mathbf{k}') \end{bmatrix} = 0$$

As we did for for the Klein-Gordon field, we could go on to construct the Poincaré currents, writing the energy, momentum and angular momentum in terms of the creation and anihilation operators. These emerge much as before. However, for the charged scalar field, there is an additional symmetry.

Exercise: Find the Hamiltonian operator

$$\hat{H} = \int : \left(\pi^* \pi + \nabla \varphi^* \cdot \nabla \hat{\varphi} + m^2 \hat{\varphi}^* \hat{\varphi}\right) : d^3 x$$

in terms of the creation and annihilation operators.

2.4 Noether current and current operator

The transformation

$$\begin{aligned} \varphi(\mathbf{x},t) &\to e^{i\alpha}\varphi(\mathbf{x},t) \\ \varphi^*(\mathbf{x},t) &\to e^{-i\alpha}\varphi^*(\mathbf{x},t) \end{aligned} \tag{41}$$

leaves the action, Eq.(??), invariant, so the complex scalar field has a global U(1) symmetry. Therefore, there is an additional Noether current. In this case, the variation of the Lagrangian, Eq.(25), under the U(1) symmetry is also zero, so from eq.(??) the Noether current is simply

$$J^{\mu} \equiv \frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \phi^{A}\right)} \Delta^{A}$$

where

$$\phi^A \rightarrow \phi^A + \Delta^A \left(\phi^B, x \right)$$

defines the infinitesimal transformation Δ^A . For an infinitesimal phase change, $e^{i\alpha} \approx 1 + i\alpha$ so the fields change by

$$\begin{array}{rcl} \varphi & \rightarrow & \varphi + i\alpha\varphi \\ \varphi^* & \rightarrow & \varphi^* - i\alpha\varphi^* \end{array}$$

so the current is

$$J^{\alpha} \equiv \frac{\partial \mathcal{L}}{\partial (\partial_{\alpha} \phi)} \Delta \varphi + \frac{\partial \mathcal{L}}{\partial (\partial_{\alpha} \phi^{*})} \Delta \varphi^{*}$$

= $(\partial^{\alpha} \varphi^{*}) i \alpha \varphi - (\partial^{\alpha} \varphi) i \alpha \varphi^{*}$
= $i \alpha \left((\partial^{\alpha} \varphi^{*}) \varphi - (\partial^{\alpha} \varphi) \varphi^{*} \right)$ (42)

We are guaranteed that the divergence of J^{α} must vanish and can easily check using the field equations:

$$\begin{aligned} \partial_{\alpha}J^{\alpha} &= i\alpha\partial_{\alpha}\left(\left(\partial^{\alpha}\varphi^{*}\right)\varphi - \left(\partial^{\alpha}\varphi\right)\varphi^{*}\right) \\ &= i\alpha\left(\left(\partial_{\alpha}\partial^{\alpha}\varphi^{*}\right)\varphi - \left(\partial^{\alpha}\varphi\right)\left(\partial_{\alpha}\varphi^{*}\right) + \left(\partial^{\alpha}\varphi^{*}\right)\left(\partial_{\alpha}\varphi\right) - \left(\partial_{\alpha}\partial^{\alpha}\varphi\right)\varphi^{*}\right) \\ &= -i\alpha\left(\frac{m^{2}}{\hbar^{2}}\varphi^{*}\varphi - \frac{m^{2}}{\hbar^{2}}\varphi\varphi^{*}\right) \\ &= 0 \end{aligned}$$

In general, when new fields are introduced to make a global symmetry into a local symmetry, the new fields produce interactions between the original, symmetric fields. The strength of this interaction is governed by the Noether currents of the symmetry. In the present case, when this U(1) (phase) invariance is gauged to produce an interaction, the new field that is introduced is the photon field, and it is this current J^{α} that carries the electric charge. Therefore, writing e for α , and writing the 4-current as $J^{\alpha} = (\rho, \mathbf{J})$, we see that

$$\rho = ie \left(\partial_0 \varphi^* \varphi - \partial_0 \varphi \varphi^*\right) \tag{43}$$

$$\mathbf{J} = ie\left(\varphi \nabla \varphi^* - \varphi^* \nabla \varphi\right) \tag{44}$$

2.5 Conserved charge operator

Classically, the spatial integral of the charge density ρ gives us conserved charge,

$$Q = \int J^0 d^3 x$$
$$= \int \rho d^3 x$$

While all of the current may be expressed in terms of operators on quantum states, we will be particuarly interested in the total charge. Substituting the operator expressions for the fields, we find that the conserved charge is given by

$$\begin{aligned} \hat{Q} &= \int :\hat{\rho}: d^{3}x \\ &= ie \int :(\partial_{0}\hat{\varphi}^{*}\hat{\varphi} - \partial_{0}\hat{\varphi}\hat{\varphi}^{*}): d^{3}x \\ &= ie \int (\hat{\pi}\hat{\varphi} - \hat{\pi}^{*}\hat{\varphi}^{*}) d^{3}x \end{aligned}$$

Substituting the fields from Eqs.(33) - (36), this becomes

$$\begin{split} \hat{Q} &= -\frac{e}{(2\pi)^3} \int d^3x : \left(\int \sqrt{\frac{\omega}{2}} d^3k \left(\hat{b} \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right) \right) \left(\int \frac{d^3k'}{\sqrt{2\omega'}} \left(\hat{a} \left(\mathbf{k'} \right) e^{i\left(\omega't - \mathbf{k'} \cdot \mathbf{x} \right)} + \hat{b}^{\dagger} \left(\mathbf{k'} \right) e^{-i\left(\omega't - \mathbf{k'} \cdot \mathbf{x} \right)} \right) \\ &- \left(\hat{a} \leftrightarrow \hat{b} \text{ and } \hat{a}^{\dagger} \leftrightarrow \hat{b}^{\dagger} \right) \\ &= -\frac{e}{2(2\pi)^3} \int d^3x \int d^3k \int d^3k' \sqrt{\frac{\omega}{\omega'}} : \left(\hat{b} \left(\mathbf{k} \right) e^{i(\omega t - \mathbf{k} \cdot \mathbf{x})} - \hat{a}^{\dagger} \left(\mathbf{k} \right) e^{-i(\omega t - \mathbf{k} \cdot \mathbf{x})} \right) \left(\hat{a} \left(\mathbf{k'} \right) e^{i\left(\omega't - \mathbf{k'} \cdot \mathbf{x} \right)} + \hat{b}^{\dagger} \left(\mathbf{k'} \right) e^{-i\left(\omega't - \mathbf{k'} \cdot \mathbf{x} \right)} \right) \\ &- \left(\hat{a} \leftrightarrow \hat{b} \text{ and } \hat{a}^{\dagger} \leftrightarrow \hat{b}^{\dagger} \right) \\ &= -\frac{e}{2(2\pi)^3} \int d^3x \int d^3k \int d^3k' \sqrt{\frac{\omega}{\omega'}} : \left[\left(\hat{b} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) e^{i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} + \mathbf{k'}\right) \cdot \mathbf{x}\right)} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) e^{-i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} \right) \\ &+ \hat{b} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k'} \right) e^{i\left(\left(\omega - \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k'} \right) e^{-i\left(\left(\omega + \omega'\right)t - \left(\mathbf{k} - \mathbf{k'}\right) \cdot \mathbf{x}\right)} \right] : \\ &- \left(\hat{a} \leftrightarrow \hat{b} \text{ and } \hat{a}^{\dagger} \leftrightarrow \hat{b}^{\dagger} \right) \end{split}$$

Integrate over d^3x , giving Dirac delta functions, $\delta(\mathbf{k} + \mathbf{k}')$ or $\delta(\mathbf{k} - \mathbf{k}')$, then integrate over d^3k' :

$$\begin{split} \hat{Q} &= -\frac{e}{2} \int d^3k \int d^3k' \sqrt{\frac{\omega}{\omega'}} : \left[\left(\hat{b} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta \left(\mathbf{k} + \mathbf{k'} \right) e^{i \left(\omega + \omega' \right) t} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k'} \right) \delta \left(\mathbf{k} - \mathbf{k'} \right) e^{-i \left(\omega - \omega' \right) t} \right) \right. \\ &+ \hat{b} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k'} \right) \delta \left(\mathbf{k} - \mathbf{k'} \right) e^{i \left(\omega - \omega' \right) t} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k'} \right) \delta \left(\mathbf{k} + \mathbf{k'} \right) e^{-i \left(\omega + \omega' \right) t} \right] : \\ &- \left(\hat{a} \leftrightarrow \hat{b} \text{ and } \hat{a}^{\dagger} \leftrightarrow \hat{b}^{\dagger} \right) \\ &= -\frac{e}{2} \int d^3k : \left[\hat{b} \left(\mathbf{k} \right) \hat{a} \left(-\mathbf{k} \right) e^{2i\omega t} - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{b} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k} \right) - \hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(-\mathbf{k} \right) e^{-2i\omega t} \right] : \\ &+ \frac{e}{2} \int d^3k : \left[\hat{a} \left(\mathbf{k} \right) \hat{b} \left(-\mathbf{k} \right) e^{2i\omega t} - \hat{b}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) - \hat{b}^{\dagger} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(-\mathbf{k} \right) e^{-2i\omega t} \right] : \end{split}$$

Noticing that changing variable $\mathbf{k} \to -\mathbf{k}$ produces

$$\iiint_{-\infty}^{\infty} d^3k \, \hat{b}\left(\mathbf{k}\right) \hat{a}\left(-\mathbf{k}\right) e^{2i\omega t} = \iiint_{-\infty}^{\infty} d^3k \, \hat{b}\left(-\mathbf{k}\right) \hat{a}\left(\mathbf{k}\right) e^{2i\omega t}$$

shows that the two $e^{2i\omega t}$ terms cancel, as do the final two $e^{-2i\omega t}$ terms. This leaves

$$\hat{Q} = -\frac{e}{2} \int d^3k : \left[-\hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) + \hat{b} \left(\mathbf{k} \right) \hat{b}^{\dagger} \left(\mathbf{k} \right) + \hat{b}^{\dagger} \left(\mathbf{k} \right) \hat{b} \left(\mathbf{k} \right) - \hat{a} \left(\mathbf{k} \right) \hat{a}^{\dagger} \left(\mathbf{k} \right) \right] :$$

Normal ordering, we have

$$\hat{Q} = e \int d^3k \left[\hat{a}^{\dagger} \left(\mathbf{k} \right) \hat{a} \left(\mathbf{k} \right) - \hat{b}^{\dagger} \left(\mathbf{k} \right) \hat{b} \left(\mathbf{k} \right) \right]$$

Writing this in terms of number operators gives a new insight. Defining

$$\hat{N}_{a} (\mathbf{k}) \equiv \hat{a}^{\dagger} (\mathbf{k}) \hat{a} (\mathbf{k}) \hat{N}_{b} (\mathbf{k}) \equiv \hat{b}^{\dagger} (\mathbf{k}) \hat{b} (\mathbf{k})$$

and acting on various states we find that these count the number of *a*-type and *b*-type particles at any given \mathbf{k} , respectively. If we integrate over \mathbf{k} we find the total number of *a*-type and *b*-type particles in a state.

In terms of number operators, the charge operator is

$$\hat{Q} = \int d^3k \left[e \hat{N}_a \left(\mathbf{k} \right) - e \hat{N}_b \left(\mathbf{k} \right) \right]$$

so the *a* and *b*-type particles have opposite charge.

It proves to be of some importance that the charge e appears as the phase of the U(1) symmetry transformation. This means that complex conjugation has the effect of changing the signs of all charges. This *charge conjugation symmetry* is one of the central discrete symmetries associated with the Lorentz group, and it plays a role when we consider the meaning of antiparticles later in this chapter. Notice, in particular, in the solution for the complex scalar field, eq.(33), that the phase of the antiparticle is just reversed from the phase for the particle.

3 Scalar multiplets

Suppose we have n scalar fields, φ^i , i = 1, ..., n governed by the action

$$S = \frac{1}{2} \int \sum \left(\partial^{\alpha} \varphi^{i} \partial_{\alpha} \varphi^{i} - m^{2} \varphi^{i} \varphi^{i} \right) d^{4}x$$

The quantization is similar to the previous cases. We find the conjugate momenta, $\pi^i = \frac{\delta L}{\delta \dot{\varphi}^i} = \dot{\varphi}^i$ and the Hamiltonian is

$$H = \frac{1}{2} \int \left(\pi^{i} \pi^{i} + \nabla \varphi^{i} \cdot \nabla \varphi^{i} + m^{2} \varphi^{i} \varphi^{i} \right) d^{3}x$$

The fundamental commutation relations are

$$\left[\hat{\pi}^{i}(\mathbf{x},t),\hat{\varphi}^{j}(\mathbf{x}',t)\right] = i\delta^{ij}\delta^{3}\left(\mathbf{x}-\mathbf{x}'\right)$$

with all others vanishing. These lead to creation and annihilation operators as before,

$$\left[\hat{a}^{i}(\mathbf{k}), \hat{a}^{j\dagger}(\mathbf{k}')\right] = \delta^{ij}\delta^{3}\left(\mathbf{k} - \mathbf{k}'\right)$$

and a number operator for each field,

$$\hat{N}(\mathbf{k}) = \hat{a}^{i\dagger}(\mathbf{k})\hat{a}^{i}(\mathbf{k})$$

The interesting feature of this case is the presence of a more general symmetry. The action S is left invariant by orthogonal rotations of the fields into one another. Thus, if O^i_{j} is an orthogonal transformation, we can define new fields

$$\varphi^{i\prime} = O^i_{j}\varphi^i$$

It is easy to see that the action is unchanged by such a transformation. For each infinitesimal generator of a rotation, $\left[\varepsilon_{(rs)}\right]^{ij} = \frac{1}{2} \left(\delta_r^i \delta_s^j - \delta_s^i \delta_r^j\right)$, there is a conserved Noether current found from the infinitesimal transformation,

$$\varphi^i \rightarrow \varphi^i + \left[\varepsilon_{(rs)}\right]^{ij} \varphi^j$$

Since the Lagrangian is invariant, the current is

$$J^{\alpha}_{(rs)} \equiv \frac{\partial \mathcal{L}}{\partial (\partial_{\alpha} \phi^{i})} \Delta_{(rs)} \varphi^{i}$$
$$= \partial^{\alpha} \varphi^{i} \left[\varepsilon_{(rs)} \right]^{ij} \varphi^{j}$$
$$= \varphi^{r} \partial^{\alpha} \varphi^{s} - \varphi^{s} \partial^{\alpha} \varphi^{r}$$

We are guaranteed that the divergence of J^{μ} vanishes when the field equations are satisfied.