4 Quantum Field Theory – Creation and Annihilation Operators

The Schrödinger equation for the simple harmonic oscillator is, of course

$$\hat{H}\Psi = \left(\frac{\hat{p}^2}{2m} + \tfrac{1}{2}m\omega^2\hat{x}^2\right)\Psi, \tag{4.1}$$

where $\hat{x} = x$ and $\hat{p} = -i(\partial/\partial x)$ if the wavefunction is written in the x representation, and where the operators satisfy the commutation relation $[\hat{x}, \hat{p}] = i$ coming from the classical Poisson bracket $\{x, p\} = 1$. It is possible to solve this equation by finding the x-space (or p-space) wavefunctions explicitly, obtaining the well-known result that the energy eigenstates have energies $E_n = (n + \frac{1}{2})\omega$, where n is an integer. There is, however, an alternative approach which will be very useful in quantum field theory. We define the two operators

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\hat{x} + \frac{i}{\sqrt{m\omega}}\hat{p}\right) \tag{4.2}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\hat{x} - \frac{i}{\sqrt{m\omega}}\hat{p}\right). \tag{4.3}$$

It is clear from the hermiticity of $\hat{x}$ and $\hat{p}$ that $\hat{a}^\dagger$ is the Hermitian conjugate of $\hat{a}$. In terms of these operators the Hamiltonian operator $\hat{H}$ becomes

$$\hat{H} = (\hat{a}^\dagger a + \tfrac{1}{2})\omega, \tag{4.4}$$

and $\hat{a}$ and $\hat{a}^\dagger$ satisfy the commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{4.5}$$

Combining the definition of the Hamiltonian operator with the above commutation relation, it is easy to see that

$$[\hat{H}, \hat{a}] = -\omega\hat{a}, \qquad [\hat{H}, \hat{a}^\dagger] = \omega\hat{a}^\dagger. \tag{4.6}$$

We consider a state $|n\rangle$ which represents an eigenstate of $\hat{H}$ (in any representation) with energy eigenvalue E_n, i.e.

$$\hat{H}|n\rangle = E_n|n\rangle. \tag{4.7}$$

Applying $\hat{a}^\dagger$ to this equation from the left, and using the commutation relation of $\hat{H}$ and $\hat{a}^\dagger$, we obtain

$$\hat{a}^\dagger\hat{H}|n\rangle = (\hat{H}\hat{a}^\dagger - \omega\hat{a}^\dagger)|n\rangle = E_n\hat{a}^\dagger|n\rangle, \tag{4.8}$$

which leads to

$$\hat{H}(\hat{a}^\dagger|n\rangle) = (E_n + \omega)(\hat{a}^\dagger|n\rangle), \tag{4.9}$$

showing that the state$(\hat{a}^\dagger|n\rangle)$ is precisely a state with energy $E_n + \omega$. One follows exactly the same type of argument to show that $(\hat{a}|n\rangle)$ is a state with energy eigenvalue $E_n - \omega$. Hence, $\hat{a}^\dagger$ and $\hat{a}$ are known respectively as raising and lowering operators.

It is also possible to use the properties of the raising and lowering operators to obtain more information about the system. Naively, if one starts with any state, and acts with $\hat{a}$ enough times one will eventually reach negative energies. This is in fact impossible. Suppose we have a state $|-\rangle$ with negative energy E_-. From the definition of the Hamiltonian, this means that $\omega\hat{a}^\dagger a|-\rangle = (E_- - \frac{1}{2}\omega)|-\rangle$, and contracting the correctly normalised Hermitian conjugate state $\langle-|$ leads to

$$\langle-|\hat{a}^\dagger a|-\rangle = E_-/\omega - \tfrac{1}{2}. \tag{4.10}$$

This right hand side is a negative number. However, $\hat{a}|-\rangle = |\Psi\rangle$, i.e. some quantum mechanical state. Since $\hat{a}^\dagger$ is the Hermitian conjugate of $\hat{a}$ this means that

$$\langle-|\hat{a}^\dagger\hat{a}|-\rangle = \langle\Psi|\Psi\rangle, \tag{4.11}$$

i.e. the modulus squared of some quantum mechanical state. This is by definition positive, or zero if the state is identically zero, and we have a contradiction. Hence, if we continually act with the lowering operator $\hat{a}$ we must always reach some state $|0\rangle$ such that $\hat{a}|0\rangle = 0$, and all subsequent operations with $\hat{a}$ also produce zero. This is known as the ground state, i.e. the state of lowest energy of the system. Since $\hat{H} = (\hat{a}^\dagger\hat{a} + \frac{1}{2})\omega$, and $\hat{a}|0\rangle = 0$, it is clear that the energy of the ground state is $\frac{1}{2}\omega$, and not only can the energy never be negative, but it has this zero-point value.

The first excited state of the system is

$$|1\rangle = \hat{a}^\dagger|0\rangle, \tag{4.12}$$

which has energy $(1 + \frac{1}{2})\omega$ The n_{th} excited state has energy $(n + \frac{1}{2})\omega$, and is given by

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle, \tag{4.13}$$

where the prefactor guarantees the correct normalisation, i.e. that $\langle n|n\rangle = 1$. Thus, we may write the operation of the Hamiltonian on the states of the system as

$$\hat{H}|n\rangle \equiv (\hat{a}^\dagger\hat{a} + \tfrac{1}{2})\omega|n\rangle = (n + \tfrac{1}{2})\omega|n\rangle. \tag{4.14}$$

This gives us the interpretation that the energy eigenstate $|n\rangle$ is an eigenstate of the number operator $\hat{a}^\dagger\hat{a}$ with integer eigenvalue n, and that this number represents the number of quanta with energy ω which have been introduced to the ground state of the system. Hence, since $\hat{a}^\dagger$ raises the energy of the system by one unit, one may think of this in terms of it creating one quantum of energy ω. Therefore, $\hat{a}^\dagger$ is often referred to as the creation operator. Likewise, $\hat{a}$ removes a quantum of energy ω and is often referred to as the annihilation operator. In quantum field theory we can construct similar creation and annihilation operators from the operator versions of the field ϕ and its conjugate field momentum π, and in this case they can be taken to have the interpretation of creating or annihilating particles at given space-time points, or with given energy and momenta. We will see how this works below.

Let us consider the lattice Action

$$S = \int dtL = \int dt\, a^3 \sum_i \left(\frac{1}{2}\left(\frac{\partial\phi(\mathbf{x}_i,t)}{\partial t}\right)^2 - \kappa \sum_{\boldsymbol{\mu}_k} \big(\phi(\mathbf{x}_i + \boldsymbol{\mu}_k, t) - \phi(\mathbf{x}_i,t)\big)^2 - \tfrac{1}{2}\omega^2\phi_i^2(\mathbf{x}_i,t) \right). \tag{4.15}$$

We may define the particle-like momentum

$$p_i = \frac{\partial L}{\partial \dot{\phi}_i} = a^3 \dot{\phi}_i = a^3 \pi_i. \tag{4.16}$$

However, we have the usual commutation relation between particle-like momentum and coordinates

$$[\phi_i, p_l] = i\delta_{il}. \tag{4.17}$$

This therefore implies the commutation relation

$$[\phi_i, \pi_l] = \frac{i}{a^3}\delta_{il}, \tag{4.18}$$

between the field and the field conjugate momentum. In the limit that $\kappa = 0$ we have a direct analogy with the previous model of the simple harmonic oscillator:

$$\hat{H} = a^3 \sum_i \hat{H}_i = a^3 \sum_i \left(\tfrac{1}{2}\pi_i^2 + \tfrac{1}{2}m^2\phi_i^2\right), \tag{4.19}$$

and defining raising and lowering operators

$$\hat{a}_i = \frac{1}{\sqrt{2}}(m\phi_i + i\pi_i), \qquad \hat{a}_i^\dagger = \frac{1}{\sqrt{2}}(m\phi_i - i\pi_i), \tag{4.20}$$

we obtain the Hamiltonian

$$\hat{H}_i = \hat{a}_i^\dagger \hat{a}_i + \tfrac{1}{2}m/a^3, \tag{4.21}$$

and the commutation relation

$$[\hat{a}_i, \hat{a}_j^\dagger] = m/a^3\delta_{ij}. \tag{4.22}$$

Therefore, we can think of $\hat{a}_i^\dagger$ and $\hat{a}_i$ as creating and destroying quanta at site i. However, we also have the interaction part of the Hamiltonian

$$\hat{H}_{int} = a^3\kappa \sum_{i,\boldsymbol{\mu}_k} \big(\phi(\mathbf{x}_i + \boldsymbol{\mu}_k, t) - \phi(\mathbf{x}_i, t)\big)^2, \tag{4.23}$$

which as well as ϕ_i^2 terms contains the component

$$-2a^3\kappa \sum_{i,\boldsymbol{\mu}_k} \phi(\mathbf{x}_i + \boldsymbol{\mu}_k, t)\phi(\mathbf{x}_i, t). \tag{4.24}$$

Noting that

$$\phi_i = \frac{\hat{a}_i^\dagger + \hat{a}_i}{\sqrt{2m}} \tag{4.25}$$

this leads to a contribution to the Hamiltonian of the form

$$\tilde{H} = -\frac{a^3\kappa}{m^2} \sum_{i,\boldsymbol{\mu}_k} \left(\hat{a}_{i+\boldsymbol{\mu}_k}^\dagger + \hat{a}_{i+\boldsymbol{\mu}_k}\right)\left(\hat{a}_i^\dagger + \hat{a}_i\right). \tag{4.26}$$

So there is a term in the Hamiltonian which enables particles to be annihilated at one site and created at the next, or vice versa, i.e. it allows the movement of particles.

Hence, broadly speaking in x-space we can create and annihilate quanta, and allow them to move on the lattice. However, it is more illuminating to get rid of the lattice and also consider the situation in momentum space. At this point we will drop the hatted notation for operators. First we let the lattice spacing $\rightarrow 0$ and consider the continuum limit. In this case $\phi_i \rightarrow \phi(\mathbf{x})$ and $\pi_i \rightarrow \pi(\mathbf{x})$ (we ignore time dependence for the moment) and the commutation relation becomes

$$[\phi(\mathbf{x}), \pi(\mathbf{y})] = i\delta^3(\mathbf{x} - \mathbf{y}). \tag{4.27}$$

We may define the momentum space fields simply as the Fourier transform of the x-space fields:

$$\phi(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\tilde{\phi}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}, \tag{4.28}$$

$$\pi(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\tilde{\pi}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}, \tag{4.29}$$

with inverse transformation

$$\tilde{\phi}(\mathbf{p}) = \int d^3\mathbf{x}\phi(\mathbf{x})e^{-i\mathbf{p}\cdot\mathbf{x}}, \tag{4.30}$$

and similar for π. By considering either $[\phi(\mathbf{x}), \pi(\mathbf{y})]$ or by writing $\tilde{\phi}(\mathbf{p})$ in terms of $\phi(\mathbf{x})$ we can find the momentum space commutation relations,

$$[\tilde{\phi}(\mathbf{p}), \tilde{\pi}(\mathbf{q})] = i(2\pi)^3\delta^3(\mathbf{p} + \mathbf{q}), \tag{4.31}$$

and

$$[\tilde{\phi}(\mathbf{p}), \tilde{\phi}(\mathbf{q})] = [\tilde{\pi}(\mathbf{p}), \tilde{\pi}(\mathbf{q})] = 0. \tag{4.32}$$

Let us now construct the Hamiltonian,

$$\int d^3\mathbf{x}\,\phi^2(\mathbf{x}) = \int d^3\mathbf{x} \int\int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{d^3\mathbf{q}}{(2\pi)^3}\tilde{\phi}(\mathbf{p})\tilde{\phi}(\mathbf{q})e^{i(\mathbf{p}+\mathbf{q})\cdot\mathbf{x}} \tag{4.33}$$

$$= \int\int \frac{d^3\mathbf{p}}{(2\pi)^3}d^3\mathbf{q}\tilde{\phi}(\mathbf{p})\tilde{\phi}(\mathbf{q})\delta^3(\mathbf{p} + \mathbf{q}) \tag{4.34}$$

$$= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\tilde{\phi}(\mathbf{p})\tilde{\phi}(-\mathbf{p}), \tag{4.35}$$

and similarly

$$\int d^3\mathbf{x}\,\pi^2(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\tilde{\pi}(\mathbf{p})\tilde{\pi}(-\mathbf{p}). \tag{4.36}$$

As seen in the previous section, as we remove the lattice the term representing the interaction between neighbouring sites becomes proportional to

$$\int d^3\mathbf{x}(\boldsymbol{\nabla}\phi(\mathbf{x}))^2, \tag{4.37}$$

which upon taking the Fourier transform becomes

$$\int \frac{d^3\mathbf{p}}{(2\pi)^3}(i\mathbf{p}) \cdot (-i\mathbf{p})\tilde{\phi}(\mathbf{p})\tilde{\phi}(-\mathbf{p}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\mathbf{p}^2\tilde{\phi}(\mathbf{p})\tilde{\phi}(-\mathbf{p}). \tag{4.38}$$

Combining all these elements in the Hamiltonian we obtain the total

$$H = \tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}\left(\tilde{\pi}(\mathbf{p})\tilde{\pi}(-\mathbf{p}) + E^2(\mathbf{p})\tilde{\phi}(\mathbf{p})\tilde{\phi}(-\mathbf{p})\right), \tag{4.39}$$

where $E^2(\mathbf{p}) = \mathbf{p}^2 + m^2$ is the usual definition of the relativistic energy of a particle with mass m and momentum $\mathbf{p}$. We define the "on-shell" energy to be $E(\mathbf{p}) = +\sqrt{\mathbf{p}^2 + m^2}$.

One can now define momentum-space annihilation and creation operators

$$a_{\mathbf{p}} = E(\mathbf{p})\phi(\mathbf{p}) + i\pi(\mathbf{p}), \tag{4.40}$$

$$a^\dagger_{\mathbf{p}} = E(-\mathbf{p})\phi(-\mathbf{p}) - i\pi(-\mathbf{p}), \tag{4.41}$$

where $E(-\mathbf{p}) = E(\mathbf{p})$. These lead to the commutation relations

$$[a_{\mathbf{q}}, a^\dagger_{\mathbf{p}}] = (2\pi)^3 2E(\mathbf{p})\delta^3(\mathbf{p} - \mathbf{q}), \tag{4.42}$$

and

$$[a_{\mathbf{q}}, a_{\mathbf{p}}] = [a^\dagger_{\mathbf{q}}, a^\dagger_{\mathbf{p}}] = 0. \tag{4.43}$$

Since these commutation relations are of the same general form as those for the quantum mechanical simple harmonic oscillator they have the same sort of interpretation. The only difference is that they are now defined for a continuum and the commutation relations between $a_{\mathbf{q}}$ and $a^\dagger_{\mathbf{p}}$ has the energy on the right hand side.

To see that these operators do indeed have the same type of interpretation we can examine their properties. Firstly we look at their relationship to the Hamiltonian. To do this we consider the combination

$$a^\dagger_{\mathbf{p}}a_{\mathbf{p}} = \left(\tilde{\pi}(\mathbf{p})\tilde{\pi}(-\mathbf{p}) + E^2(\mathbf{p})\tilde{\phi}(\mathbf{p})\tilde{\phi}(-\mathbf{p}) + iE(\mathbf{p})\big(\tilde{\phi}(-\mathbf{p})\tilde{\pi}(\mathbf{p}) - \tilde{\pi}(-\mathbf{p})\tilde{\phi}(\mathbf{p})\big)\right). \tag{4.44}$$

From this we see that

$$\tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}a^\dagger_{\mathbf{p}}a_{\mathbf{p}} = H + \tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}iE(\mathbf{p})\big(\tilde{\phi}(-\mathbf{p})\tilde{\pi}(\mathbf{p}) - \tilde{\pi}(-\mathbf{p})\tilde{\phi}(\mathbf{p})\big)\Big), \tag{4.45}$$

and letting $\mathbf{p} \to -\mathbf{p}$ in the second term in the integral

$$\tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}a^\dagger_{\mathbf{p}}a_{\mathbf{p}} = H + \tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}iE(\mathbf{p})[\tilde{\phi}(-\mathbf{p}), \tilde{\pi}(\mathbf{p})]. \tag{4.46}$$

Using the known commutation relation we therefore get

$$H = \tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3}a^\dagger_{\mathbf{p}}a_{\mathbf{p}} + \tfrac{1}{2}\delta^3(0)\int d^3\mathbf{p}E(\mathbf{p}). \tag{4.47}$$

Hence, the Hamiltonian is the integral over all $a_{\mathbf{p}}^\dagger a_{\mathbf{p}}/2$ terms but also the sum over the zero point energy for an infinite number of oscillators in the system.

One could also write the Hamiltonian in the equivalent form

$$H = \tfrac{1}{4}\int \frac{d^3\mathbf{p}}{(2\pi)^3}\big(a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{\mathbf{p}} a_{\mathbf{p}}^\dagger\big). \tag{4.48}$$

This allows a convenient way of eliminating this infinite, but unphysical zero-point energy. We define a normal-ordered operator, denoted by $: A :$ as one where we take the operator A and write all annihilation operators to the right of all creation operators. Hence, by definition

$$: H := \tfrac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} = \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}\, E(\mathbf{p}) a_{\mathbf{p}}^\dagger a_{\mathbf{p}}. \tag{4.49}$$

Where in the expression on the right hand side we have separated the integral out into a phase space integral $\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}$ and the integrand $E(\mathbf{p})a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$. This normal-ordered Hamiltonian now ignores the ground state energy. The separation into the phase space and integrand occurs because $\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}$ is a Lorentz invariant space space in our standard four-dimensional space time. To see this we consider that the full expression for the four-dimensional integration for real particles is

$$\int \frac{d^3\mathbf{p}\, dE(\mathbf{p})}{(2\pi)^3}\delta^+(E^2(\mathbf{p}) - \mathbf{p}^2 - m^2), \tag{4.50}$$

where the delta function enforces that the particle satisfies $E^2(\mathbf{p}) - \mathbf{p}^2 - m^2$ and specifies that the positive energy solution should be taken. We can write the delta function as

$$\delta^+\bigg((E(\mathbf{p}) - \sqrt{\mathbf{p}^2+m^2})(E(\mathbf{p}) + \sqrt{\mathbf{p}^2+m^2})\bigg) \equiv \frac{1}{E(\mathbf{p}) + \sqrt{\mathbf{p}^2+m^2}}\delta((E(\mathbf{p}) - \sqrt{\mathbf{p}^2+m^2}). \tag{4.51}$$

Performing the integral over $E(\mathbf{p})$ we replace $1/(E(\mathbf{p})+\sqrt{\mathbf{p}^2+m^2})$ by $1/(2E(\mathbf{p}))$ and eliminate the delta function and

$$\int \frac{d^3\mathbf{p}\, dE(\mathbf{p})}{(2\pi)^3}\delta^+(E^2(\mathbf{p}) - \mathbf{p}^2 - m^2) \to \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}. \tag{4.52}$$

So our expression for the Hamiltonian is the integral of $E(\mathbf{p})a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$ over the Lorentz-invariant phase space.

We can now consider the action of the operators $a_{\mathbf{p}}^\dagger$ and $a_{\mathbf{p}}$. Let us define a state vector

$$|\Psi\rangle = |n_1, n_2, \ldots\rangle, \tag{4.53}$$

where n_j is the number of particles with momentum $\mathbf{p}_j$. For this state $H|\Psi\rangle = E|\Psi\rangle$. We also define the state $|\Psi'\rangle = a_{\mathbf{p}}^\dagger|\Psi\rangle$, and consider the way in which the Hamiltonian acts on this.

$$\begin{aligned} H|\Psi'\rangle &= \tfrac{1}{2}\int \frac{d^3\mathbf{q}}{(2\pi)^3} a_{\mathbf{q}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}}^\dagger|\Psi\rangle \\ &= \tfrac{1}{2}\int \frac{d^3\mathbf{q}}{(2\pi)^3} a_{\mathbf{q}}^\dagger\big(a_{\mathbf{p}}^\dagger a_{\mathbf{q}} + (2\pi)^3 2E(\mathbf{p})\delta^3(\mathbf{p}-\mathbf{q})\big)|\Psi\rangle \\ &= a_{\mathbf{p}}^\dagger E|\Psi\rangle + a_{\mathbf{p}}^\dagger E(\mathbf{p})|\Psi\rangle \\ &= (E + E(\mathbf{p}))|\Psi'\rangle. \end{aligned} \tag{4.54}$$

This means that the operator $a_{\mathbf{p}}^\dagger$ creates a particle with specific momentum $\mathbf{p}$ and "on-shell" energy $E^2(\mathbf{p}) = \mathbf{p}^2 + m^2$. By a similar argument one finds that $a_{\mathbf{p}}$ annihilates such a particle. The ground state is then defined by $a_{\mathbf{p}}|0\rangle = 0$ for all $\mathbf{p}$ and hence by definition $: H : |0\rangle = 0$.

5 Commutators and Time Dependence

In the last section we were able to define the Hamiltonian for scalar field theory in terms of creation and annihilation operators $a^\dagger_{\mathbf{p}}$ and $a_{\mathbf{p}}$ which can be related to the momentum-space field by

$$\tilde{\phi}(\mathbf{p}) = \frac{a_{\mathbf{p}} + a^\dagger_{-\mathbf{p}}}{2E(\mathbf{p})}. \tag{5.1}$$

Hence, by taking the Fourier transform to x-space we obtain

$$\phi(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}}(a_{\mathbf{p}} + a^\dagger_{-\mathbf{p}}), \tag{5.2}$$

on letting $\mathbf{p} \to -\mathbf{p}$ in the second term

$$\phi(\mathbf{x}) = \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}((a_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{x}}). \tag{5.3}$$

Similarly

$$\pi(\mathbf{x}) = i\int \frac{d^3\mathbf{p}}{2(2\pi)^3}((-a_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} + a^\dagger_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{x}}), \tag{5.4}$$

and by construction the fields defined in this way must satisfy the coordinate space commutation relation $[\phi(\mathbf{x}), \pi(\mathbf{y})] = i\delta^3(\mathbf{x} - \mathbf{y})$.

This is all very well, but as yet takes no account of time dependence, and is also for a non-interacting theory, i.e. we simply consider the creation and annihilation of particles with no interaction between them. We will first discuss the time dependence since this is necessary before looking at interacting theories. This requires the introduction of different pictures in quantum theories.

Usually in quantum mechanics we work in the Schrödinger picture. In this the operators are constant in time and the state vectors evolve:

$$\frac{dQ}{dt} = 0 \qquad\qquad i\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle, \tag{5.5}$$

and solving the latter

$$|\Psi, t\rangle = e^{-iH(t-t_0)}|\Psi, t_0\rangle. \tag{5.6}$$

However, physical results, e.g. expectation values $\langle\Psi|Q|\Psi\rangle$ allow a change of time dependence. In particular, in the Heisenberg picture all time dependence goes into the operators, i.e.

$$\begin{aligned} \langle\Psi, t|_S Q_S|\Psi, t\rangle_S &= \langle\Psi, t_0|e^{+iH(t-t_0)}(Q(t_0))e^{-iH(t-t_0)}|\Psi, t_0\rangle & (5.7)\\ \to \langle\Psi|_H Q_H(t)|\Psi\rangle_H &= \langle\Psi, t_0|(e^{+iH(t-t_0)}Q(t_0)e^{-iH(t-t_0)})|\Psi, t_0\rangle. & (5.8) \end{aligned}$$

Therefore, in this picture

$$i\frac{dQ_H}{dt} = [Q_H, H], \tag{5.9}$$

i.e. we obtain the analogy of the Poisson bracket equation for time evolution at the operator level without having to take expectation values.

It is often most convenient to define a quantum field theory in the Heisenberg picture in which case the operators evolve with time while the state vector is time-independent, and simply specifies the number of particles with given momentum in the state. In the Heisenberg picture it is clear that $dH/dt = 0$ since $[H, H] = 0$, and this is true for a variety of other operators such as the number operator or momentum operator which are simply related to H. However, for the quantum fields ϕ and π it is not so simple. Each of these is a linear combination of $a_{\mathbf{p}}^\dagger$ and $a_{\mathbf{p}}$. Hence, we need to know

$$e^{+iHt} a_{\mathbf{p}}^\dagger e^{-iHt} \qquad \text{and} \qquad e^{+iHt} a_{\mathbf{p}} e^{-iHt} \tag{5.10}$$

where e^{iHt} represents the formal definition (since H is an operator)

$$e^{iHt} = 1 + iHt + (iHt)^2/2 + \cdots . \tag{5.11}$$

To move $a_{\mathbf{p}}^\dagger$ through e^{iHt} we need to consider $a_{\mathbf{p}}^\dagger H$.

$$a_{\mathbf{p}}^\dagger H = \int \frac{d^3\mathbf{q}}{2(2\pi)^3} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{q}} = \int \frac{d^3\mathbf{q}}{2(2\pi)^3} a_{\mathbf{q}}^\dagger a_{\mathbf{p}}^\dagger a_{\mathbf{q}}. \tag{5.12}$$

But using the commutation relation $a_{\mathbf{p}}^\dagger a_{\mathbf{q}} = a_{\mathbf{q}} a_{\mathbf{p}}^\dagger - 2E(\mathbf{p})(2\pi)^3 \delta^3(\mathbf{p} - \mathbf{q})$ we obtain

$$a_{\mathbf{p}}^\dagger H = H a_{\mathbf{p}}^\dagger - E(\mathbf{p}) a_{\mathbf{p}}^\dagger = (H - E(\mathbf{p})) a_{\mathbf{p}}^\dagger. \tag{5.13}$$

Repeating this procedure we find

$$e^{+iHt} a_{\mathbf{p}}^\dagger e^{-iHt} = e^{+iHt} e^{-i(H - E(\mathbf{p}))t} a_{\mathbf{p}}^\dagger = e^{+iE(\mathbf{p})t} a_{\mathbf{p}}^\dagger. \tag{5.14}$$

Using an analogous argument we also find that

$$e^{+iHt} a_{\mathbf{p}} e^{-iHt} = e^{-iE(\mathbf{p})t} a_{\mathbf{p}}, \tag{5.15}$$

and therefore,

$$\begin{aligned}
\phi_H(\mathbf{x}, t) &= e^{iHt} \phi_S(\mathbf{x}) e^{-iHt} \\
&= \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3} (a_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x} - iE(\mathbf{p})t} + a_{\mathbf{p}}^\dagger e^{-i\mathbf{p}\cdot\mathbf{x} + iE(\mathbf{p})t}) \\
&= \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3} (a_{\mathbf{p}} e^{-ip\cdot x} + a_{\mathbf{p}}^\dagger e^{ip\cdot x}).
\end{aligned} \tag{5.16}$$

And in the same manner we find

$$\pi_H(\mathbf{x}, t) = i \int \frac{d^3\mathbf{p}}{2(2\pi)^3} (-a_{\mathbf{p}} e^{-ip\cdot x} + a_{\mathbf{p}}^\dagger e^{ip\cdot x}). \tag{5.17}$$

Hence, $\pi_H = d\phi_H/dt$, the same as the classical relation between the field and its conjugate momentum. Also we note that both $\phi_H(x)$ and $\pi_H(x)$ satisfy the Klein-Gordon equation and that the part $\propto a_{\mathbf{p}}^\dagger$ corresponds to the negative energy solutions, while that $\propto a_{\mathbf{p}}$ corresponds to the positive frequency solutions.

Now that we have the time-dependent field operators we can examine the unequal time commutators. We know that $[\phi(\mathbf{x},t),\phi(\mathbf{y},t)] = 0$ but there are certain properties which must be satisfied by $[\phi(\mathbf{x},t_1),\phi(\mathbf{y},t_2)]$. In particular, we want the fields, and their commutation relations to be Lorentz invariant, and in order to be consistent with special relativity we want fields with a space-like separation to have a vanishing commutation relation. We can check this in detail.

$$\begin{aligned}
[\phi(x),\phi(y)] &= \int\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}\frac{d^3\mathbf{q}}{2E(\mathbf{q})(2\pi)^3}[(a_{\mathbf{p}}e^{-ip\cdot x}+a^\dagger_{\mathbf{p}}e^{ip\cdot x}),(a_{\mathbf{q}}e^{-iq\cdot y}+a^\dagger_{\mathbf{q}}e^{iq\cdot y})] \\
&= \int\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}\frac{d^3\mathbf{q}}{2E(\mathbf{q})(2\pi)^3}([a^\dagger_{\mathbf{p}},a_{\mathbf{q}}]e^{ip\cdot x-iq\cdot y}+[a_{\mathbf{p}},a^\dagger_{\mathbf{q}}]e^{iq\cdot y-ip\cdot x}) \\
&= \int\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}d^3\mathbf{q}\delta^3(\mathbf{p}-\mathbf{q})(-e^{ip\cdot x-iq\cdot y}+e^{iq\cdot y-ip\cdot x}) \\
&= \int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}(e^{-ip\cdot(x-y)}-e^{ip\cdot(x-y)}) \\
&= i\Delta(x-y). \qquad (5.18)
\end{aligned}$$

This unequal time commutator is now not always zero. However, since we have a Lorentz invariant phase space it is Lorentz invariant, i.e. a function of $(x-y)^2$. If $t_1 = t_2$ we have the situation of the equal time commutator, i.e. $\Delta(\mathbf{x}-\mathbf{y},0) = 0$. By considering all possible values of $(\mathbf{x}-\mathbf{y})^2$ we can obtain all possible space-like values of $(x-y)^2$, i.e. all space-like separations of the two fields, and hence $\Delta(x-y) = 0$ for space-like separations. So using the Lorentz invariance we see that $[\phi(\mathbf{x},t_1),\phi(\mathbf{y},t_2)] = 0$ for all space-like separations and causality is respected, i.e. the fields do not influence each other if their positions are outside each other's light-cones.

We can consider a time-like separation by putting $\mathbf{x} = \mathbf{y}$ and looking at all possible values of $(t_1-t_2)^2$, thus generating all possible $(x-y)^2 > 0$. In this case

$$\begin{aligned}
\Delta(x-y) &= -i\int \frac{d^3\mathbf{p}}{2E(\mathbf{p})(2\pi)^3}(e^{-iE(\mathbf{p})\cdot(t_1-t_2)}-e^{iE(\mathbf{p})\cdot(t_1-t_2)}) \\
&= \int \frac{d^3\mathbf{p}}{E(\mathbf{p})(2\pi)^3}\sin\big(E(\mathbf{p})\cdot(t_2-t_1)\big), \qquad (5.19)
\end{aligned}$$

which is not equal to 0 in general.