4
Canonical Quantization

We will now begin the discussion of our main subject of interest: the role of quantum mechanical fluctuations in systems with infinitely many degrees of freedom. We will begin with a brief overview of quantum mechanics of a single particle.

4.1 Elementary Quantum Mechanics

Elementary Quantum Mechanics describes the quantum dynamics of systems with a finite number of degrees of freedom. Two axioms are involved in the standard procedure for quantizing a classical system. Let $L(q, \dot{q})$ be the Lagrangian of an abstract dynamical system described by the generalized coordinate q. In Chapter two, we recalled that the canonical formalism of Classical Mechanics is based on the concept of canonical pairs of dynamical variables. So, the canonical coordinate q has for partner the canonical momentum p:

$$p = \frac{\partial L}{\partial \dot{q}} \tag{4.1}$$

In the canonical formalism, the dynamics of the system is governed by the classical Hamiltonian

$$H(q, p) = p\dot{q} - L(q, \dot{q}) \tag{4.2}$$

which is the Legendre transform of the Lagrangian. In the canonical (Hamiltonian) formalism the equations of motion are just Hamilton's Equations,

$$\dot{p} = -\frac{\partial H}{\partial q} \qquad \dot{q} = \frac{\partial H}{\partial p} \tag{4.3}$$

The dynamical state of the system is defined by the values of the canonical coordinates and momenta at any given time t. As a result of these definitions, the coordinates and momenta satisfy a set of Poisson Bracket relations

$$\{q,p\}_{PB} = 1 \qquad \{q,q\}_{PB} = \{p,p\}_{PB} = 0 \tag{4.4}$$

where

$$\{A,B\}_{PB} \equiv \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} \tag{4.5}$$

In Quantum Mechanics, the primitive (or fundamental) notion is the concept of a *physical state.* A physical state of a system is a represented by a *state vector* in an abstract vector space, which is called the Hilbert space $\mathcal{H}$ of quantum states. The space $\mathcal{H}$ is a vector space in the sense that if two vectors $|\Psi\rangle \in \mathcal{H}$ and $|\Phi\rangle \in \mathcal{H}$ represent physical states, then the *linear superposition* $|a\Psi + b\Phi\rangle = a|\Psi\rangle + b|\Phi\rangle$, where a and b are two arbitrary complex numbers, also represents a physical state and thus it is an element of the Hilbert space i.e. $|a\Psi + b\Phi\rangle \in \mathcal{H}$. The *Superposition Principle* is an axiom of Quantum Mechanics.

In Quantum Mechanics, the dynamical variables, i.e. the generalized coordinates, $\hat{q}$, and the associated canonical momenta $\hat{p}$, the Hamiltonian H, etc., are represented by *operators* that act *linearly* on the Hilbert space of states. Hence, Quantum Mechanics is a linear theory, even though the physical observables obey non-linear Heisenberg equations of motion. Let us denote by $\hat{A}$ an arbitrary operator acting on the Hilbert space $\mathcal{H}$. The result of acting on the state $|\Psi\rangle \in \mathcal{H}$ with the operator $\hat{A}$ is another state $|\Phi\rangle \in \mathcal{H}$,

$$\hat{A}|\Psi\rangle = |\Phi\rangle \tag{4.6}$$

The Hilbert space $\mathcal{H}$ is endowed with an *inner product.* An inner product is an operation that assigns a complex number $\langle\Phi|\Psi\rangle$ to a given pair of states $|\Phi\rangle \in \mathcal{H}$ and $|\Psi\rangle \in \mathcal{H}$.

Since $\mathcal{H}$ is a vector space, there exists a set of linearly independent states $\{|\lambda\rangle\}$, called a *basis,* that spans the entire Hilbert space. Thus, an arbitrary state $|\Psi\rangle$ can be expanded as a linear combination of a complete set of states that form a basis of $\mathcal{H}$,

$$|\Psi\rangle = \sum_{\lambda} \Psi_\lambda\, |\lambda\rangle \tag{4.7}$$

which is unique for a fixed set of basis states. The basis states can be chosen to be *orthonormal* with respect to the inner product,

$$\langle\lambda|\mu\rangle = \delta_{\lambda\mu} \tag{4.8}$$

In general, if $|\Psi\rangle$ and $|\Phi\rangle$ are normalized states

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1 \tag{4.9}$$

the action of an operator $\hat{A}$ on a state $|\Psi\rangle$ is proportional to a (generally different) state $|\Phi\rangle$,

$$\hat{A}|\Psi\rangle = \alpha|\Phi\rangle \tag{4.10}$$

The coefficient α is a complex number that depends on the pair of states and on the operator $\hat{A}$. This coefficient is the *matrix element* of $\hat{A}$ between the state $|\Psi\rangle$ and $|\Phi\rangle$, which we write with the notation

$$\alpha = \langle\Phi|\hat{A}|\Psi\rangle \tag{4.11}$$

Operators that act on a Hilbert space do not generally commute with each other. One of the axioms of Quantum Mechanics is the *Correspondence Principle* which states that in the classical limit, $\hbar \to 0$, the operators should effectively become numbers, and commute with each other in the classical limit.

The procedure of *canonical quantization* consists in demanding that to the classical canonical pair (q, p), that satisfies the Poisson Bracket $\{q, p\}_{PB} = 1$, we associate a *pair of operators* $\hat{q}$ and $\hat{p}$, acting on the Hilbert space of states $\mathcal{H}$, which obey the *canonical commutation relations*

$$[\hat{q}, \hat{p}] = i\hbar \qquad [\hat{q}, \hat{q}] = [\hat{p}, \hat{p}] = 0 \tag{4.12}$$

Here $[\hat{A}, \hat{B}]$ is the commutator of the operators $\hat{A}$ and $\hat{B}$,

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{4.13}$$

In particular, two operators that do not commute with each other cannot be diagonalized simultaneously. Hence, it is not possible to measure simultaneously with arbitrary precision in the same physical state two non-commuting observables. This is the the *Uncertainty Principle*.

By following this prescription, we assign to the classical Hamiltonian $H(q, p)$, which is a *function* of the dynamical variables q and p, an *operator* $\hat{H}(\hat{q}, \hat{p})$ obtained by replacing the dynamical variables with the corresponding operators. Other classical dynamical quantities are similarly associated in Quantum Mechanics with quantum operators that act on the Hilbert space of states. Moreover, all operators associated with classical physical quantities, in Quantum Mechanics are *hermitian operators* relative to the inner product defined in the Hilbert space $\mathcal{H}$. Namely, if $\hat{A}$ is an operator and $\hat{A}^\dagger$ is the *adjoint* of $\hat{A}$

$$\langle\Psi|\hat{A}^\dagger|\Phi\rangle \equiv \langle\Phi|\hat{A}\Psi\rangle^*, \tag{4.14}$$

then, $\hat{A}$ is hermitian iff $\hat{A} = \hat{A}^\dagger$ (with suitable boundary conditions).

The quantum mechanical state of the system at time t, $|\Psi(t)\rangle$, obeys the Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} \, |\Phi(t)\rangle = \hat{H}(\hat{q}, \hat{p}) \, |\Psi(t)\rangle \tag{4.15}$$

The state $|\Psi(t)\rangle$ is uniquely determined by the initial state $|\Psi(0)\rangle$. Thus, in Quantum Mechanics, just as in Classical Mechanics, the Hamiltonian is the generator of the (infinitesimal) time evolution of the state of a physical system.

It is always possible to choose a basis in which a particular operator is diagonal. For instance, if the operator is the canonical coordinate $\hat{q}$, a possible set of basis states are labelled by q and are its eigenstates, i.e.

$$\hat{q}|q\rangle = q \, |q\rangle \tag{4.16}$$

The basis states $\{|q\rangle\}$ are *orthonormal* and *complete*,

$$\langle q|q'\rangle = \delta(q - q'), \qquad \hat{I} = \int dq \, |q\rangle\langle q| \tag{4.17}$$

A state vector $|\Psi\rangle$ can be expanded in an arbitrary basis. If the basis of states is $\{|q\rangle\}$, the expansion is

$$|\Psi\rangle = \sum_q \Psi(q) \, |q\rangle \equiv \int_{-\infty}^{+\infty} dq \; \Psi(q) \, |q\rangle \tag{4.18}$$

where we used that the eigenvalues of the coordinate q are the real numbers. The coefficients $\Psi(q)$ of this expansion

$$\Psi(q) = \langle q|\Psi\rangle, \tag{4.19}$$

i.e. the amplitude to find the system at coordinate q in this state, are the values of the *wave function* of the state $|\Psi\rangle$ in the *coordinate representation.*

Since the canonical momentum $\hat{p}$ does not commute with $\hat{q}$, it is not diagonal in this representation. Just as in Classical Mechanics, in Quantum Mechanics too the momentum operator $\hat{p}$ is the *generator of infinitesimal displacements*. Consider the states $|q\rangle$ and $\exp(-\frac{i}{\hbar} a\hat{p}) \, |q\rangle$. It is easy to prove that the latter is the state $|q + a\rangle$ since

$$\hat{q} \; \exp\Big(- \frac{i}{\hbar} a\hat{p}\Big) \, |q\rangle \equiv \hat{q} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-ia}{\hbar} \right)^n \; \hat{p}^n \, |q\rangle \tag{4.20}$$

Using the commutation relation $[\hat{q}, \hat{p}] = i\hbar$, it is easy to show that

$$[\hat{q}, \hat{p}^n] = i\hbar n \hat{p}^{n-1} \tag{4.21}$$

Hence, we can write

$$\hat{q}\ \exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle = (q+a)\exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle \tag{4.22}$$

Thus,

$$\exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle = |q+a\rangle \tag{4.23}$$

This is a unitary transformation, i.e.

$$\left(\exp\left(-\frac{i}{\hbar}a\hat{p}\right)\right)^{-1} = \left(\exp\left(-\frac{i}{\hbar}a\hat{p}\right)\right)^{\dagger} \tag{4.24}$$

We can now use this property to compute the matrix element

$$\langle q|\exp\left(\frac{i}{\hbar}a\hat{p}\right)|\Psi\rangle \equiv \Psi(q+a) \tag{4.25}$$

For a infinitesimally small, it can be approximated by

$$\Psi(q+a) \approx \Psi(q) + \frac{i}{\hbar}a\langle q|\hat{p}|\Psi\rangle + \dots \tag{4.26}$$

We find that the matrix element for $\hat{p}$ has to satisfy

$$\langle q|\hat{p}|\Psi\rangle = \frac{\hbar}{i}\lim_{a\to 0}\frac{\Psi(q+a)-\Psi(q)}{a} \tag{4.27}$$

Thus, the operator $\hat{p}$ is represented by a differential operator

$$\langle q|\hat{p}|\Psi\rangle \equiv \frac{\hbar}{i}\frac{\partial}{\partial q}\Psi(q) = \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q|\Psi\rangle \tag{4.28}$$

It is easy to check that the coordinate representation of the operator

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial q} \tag{4.29}$$

and the coordinate operator $\hat{q}$ satisfy the commutation relation $[\hat{q},\hat{p}] = i\hbar$.

4.2 Canonical quantization in Field Theory

We will now apply the axioms of Quantum Mechanics to a Classical Field Theory. The result will be a Quantum Field Theory. For the sake of simplicity we will consider first the case of a scalar field $\phi(x)$. We have seen before that, given a Lagrangian density $\mathcal{L}(\phi,\partial_\mu\phi)$, the Hamiltonian can be found once the canonical momentum $\Pi(x)$ is defined,

$$\Pi(x) = \frac{\delta\mathcal{L}}{\delta\partial_0\phi(x)} \tag{4.30}$$

On a given time surface x_0, the classical Hamiltonian is

$$H = \int d^3x \, \left[\Pi(\boldsymbol{x}, x_0)\partial_0\phi(\boldsymbol{x}, x_0) - \mathcal{L}(\phi, \partial_\mu\phi)\right] \tag{4.31}$$

We quantize this theory by assigning to each dynamical variable of the classical theory a hermitian operator that acts on the Hilbert space of the quantum states of the system. Thus, the field $\hat{\phi}(\boldsymbol{x})$ and the canonical momentum $\widehat{\Pi}(\boldsymbol{x})$ are operators acting on a Hilbert space. These operators obey *canonical commutation relations*

$$\left[\hat{\phi}(\boldsymbol{x}), \widehat{\Pi}(\boldsymbol{y})\right] = i\hbar\delta(\boldsymbol{x} - \boldsymbol{y}) \tag{4.32}$$

In the *field representation*, the Hilbert space is the vector space of wave functions Ψ which are *functionals* of the configurations of the field (at a fixed time), which we will denote as $\{\phi(\boldsymbol{x})\}$. In this notation, the wave functionals, i.e. the amplitude to find the state of the field in a given configuration, are

$$\Psi[\{\phi(\boldsymbol{x})\}] \equiv \langle\{\phi(\boldsymbol{x})\}|\Psi\rangle \tag{4.33}$$

In this representation, the field is a diagonal operator

$$\langle\{\phi\}|\hat{\phi}(\boldsymbol{x})|\Psi\rangle \equiv \phi(\boldsymbol{x}) \, \langle\{\phi(\boldsymbol{x})\}|\Psi\rangle = \phi(\boldsymbol{x}) \, \Psi[\{\phi\}] \tag{4.34}$$

The canonical momentum $\widehat{\Pi}(\boldsymbol{x})$ is not diagonal in this representation but acts on the wave functionals as a functional differential operator,

$$\langle\{\phi\}|\widehat{\Pi}(\boldsymbol{x})|\Psi\rangle \equiv \frac{\hbar}{i}\frac{\delta}{\delta\phi(\boldsymbol{x})}\Psi[\{\phi\}] \tag{4.35}$$

What we just described is the *Schrödinger Picture* of quantum field theory. In this picture, as usual, the *operators* are time-independent but the *states* are time-dependent and satisfy the Schrödinger Equation

$$i\hbar\partial_0\Psi[\{\phi\}, x_0] = \widehat{H}\Psi[\{\phi\}, x_0] \tag{4.36}$$

For the particular case of a scalar field ϕ with the classical Lagrangian $\mathcal{L}$

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 - V(\phi) \tag{4.37}$$

the quantum mechanical Hamiltonian operator $\hat{H}$ is

$$\widehat{H} = \int d^3x \, \left\{\frac{1}{2}\widehat{\Pi}^2(\boldsymbol{x}) + \frac{1}{2}(\nabla\hat{\phi}(\boldsymbol{x}))^2 + V(\boldsymbol{\phi}(\boldsymbol{x}))\right\} \tag{4.38}$$

The stationary states are the eigenstates of the Hamiltonian $\widehat{H}$.

While it is possible to proceed further with the Schrödinger picture, the manipulation of wave functionals becomes very cumbersome rather quickly. For this reason, the *Heisenberg Picture* is commonly used.

In the Schrödinger Picture the time evolution of the system is encoded in the time dependence of the states. In contrast, in the Heisenberg Picture the operators are time-dependent while the states are time-independent. The operators of the Heisenberg Picture obey quantum mechanical equations of motion.

Let $\hat{A}$ be some operator that acts on the Hilbert space of states. Let us denote by $\hat{A}_H(x_0)$ the Heisenberg operator at time x_0, defined by

$$\hat{A}_H(x_0) = e^{\frac{i}{\hbar}\hat{H}x_0}\ \hat{A}\ e^{-\frac{i}{\hbar}\hat{H}x_0} \tag{4.39}$$

for a system with a time-independent Hamiltonian $\widehat{H}$. It is straightforward to check that $\hat{A}_H(x_0)$ obeys the equation of motion

$$i\hbar\partial_0\hat{A}_H(x_0) = [\hat{A}_H(x_0), \widehat{H}] \tag{4.40}$$

Notice that in the classical limit, the dynamical variable $A(x_0)$ obeys the classical equation of motion

$$\partial_0 A(x_0) = \{A(x_0), H\}_{PB} \tag{4.41}$$

where it is assumed that all the time dependence in A comes from the time dependence of the field (the "coordinates") and of their canonical momenta.

In the Heisenberg picture both $\hat{\phi}(\boldsymbol{x}, x_0)$ and $\widehat{\Pi}(\boldsymbol{x}, x_0)$ are time-dependent operators that obey the quantum mechanical equations of motion

$$i\hbar\partial_0\hat{\phi}(\boldsymbol{x}, x_0) = \left[\hat{\phi}(\boldsymbol{x}, x_0), \widehat{H}\right], \quad i\hbar\partial_0\widehat{\Pi}(\boldsymbol{x}, x_0) = [\widehat{\Pi}(\boldsymbol{x}, x_0), \widehat{H}] \tag{4.42}$$

The Heisenberg field operators $\hat{\phi}(\boldsymbol{x}, x_0)$ and $\widehat{\Pi}(\boldsymbol{x}, x_0)$ (we will omit the subindex "H" from now on) obey *equal-time commutation relations*

$$\left[\hat{\phi}(\boldsymbol{x}, x_0), \widehat{\Pi}(\boldsymbol{y}, x_0)\right] = i\hbar\delta(\boldsymbol{x} - \boldsymbol{y}) \tag{4.43}$$

4.3 Quantization of the free scalar field theory

We will now quantize the theory of a relativistic scalar field $\phi(x)$. In particular, we consider a *free real* scalar field ϕ whose Lagrangian density is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - \frac{1}{2}m^2\phi^2 \tag{4.44}$$

The quantum mechanical Hamiltonian $\widehat{H}$ for a free real scalar field is

$$\widehat{H} = \int d^3x \left[\frac{1}{2}\widehat{\Pi}^2(\boldsymbol{x}) + \frac{1}{2}\left(\nabla\hat{\phi}(\boldsymbol{x})\right)^2 + \frac{1}{2}m^2\hat{\phi}^2(\boldsymbol{x})\right] \tag{4.45}$$

where $\hat{\phi}$ and $\widehat{\Pi}$ satisfy the equal-time commutation relations (in units with $\hbar = c = 1$)

$$[\hat{\phi}(\boldsymbol{x}, x_0), \widehat{\Pi}(\boldsymbol{y}, x_0)] = i\delta(\boldsymbol{x} - \boldsymbol{y}) \tag{4.46}$$

In the Heisenberg representation, $\hat{\phi}$ and $\widehat{\Pi}$ are time dependent operators while the states are time independent. The field operators obey the equations of motion

$$i\partial_0\hat{\phi}(\boldsymbol{x}, x_0) = [\hat{\phi}(\boldsymbol{x}, x_0), \widehat{H}], \qquad i\partial_0\widehat{\Pi}(\boldsymbol{x}, x_0) = [\widehat{\Pi}(\boldsymbol{x}, x_0), \widehat{H}] \tag{4.47}$$

These are operator equations. After some algebra, we find that the Heisenberg equations of motion for the field and for the canonical momentum are

$$\partial_0\hat{\phi}(\boldsymbol{x}, x_0) = \widehat{\Pi}(\boldsymbol{x}, x_0) \tag{4.48}$$

$$\partial_0\widehat{\Pi}(\boldsymbol{x}, x_0) = \nabla^2 \hat{\phi}(\boldsymbol{x}, x_0) - m^2\hat{\phi}(\boldsymbol{x}, x_0) \tag{4.49}$$

Upon substitution we derive the field equation for the scalar field operator

$$\left(\partial^2 + m^2\right)\hat{\phi}(x) = 0 \tag{4.50}$$

Thus, the field operators $\hat{\phi}(x)$ satisfy the Klein-Gordon equation as their Heisenberg equation of motion.

4.3.1 Field expansions

Let us solve the field equation of motion by a Fourier transform

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3}\, \hat{\phi}(\boldsymbol{k}, x_0)\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \tag{4.51}$$

where $\hat{\phi}(\boldsymbol{k}, x_0)$ are the Fourier amplitudes of $\hat{\phi}(x)$. By demanding that the $\hat{\phi}(x)$ satisfies the Klein-Gordon equation, we find that $\hat{\phi}(\boldsymbol{k}, x_0)$ should satisfy

$$\partial_0^2\hat{\phi}(\boldsymbol{k}, x_0) + (\boldsymbol{k}^2 + m^2)\hat{\phi}(\boldsymbol{k}, x_0) = 0 \tag{4.52}$$

Also, since $\hat{\phi}(\boldsymbol{x}, x_0)$ is a real hermitian field operator, $\hat{\phi}(\boldsymbol{k}, x_0)$ must satisfy

$$\hat{\phi}^\dagger(\boldsymbol{k}, x_0) = \hat{\phi}(-\boldsymbol{k}, x_0) \tag{4.53}$$

The time dependence of $\hat{\phi}(\boldsymbol{k}, x_0)$ is trivial. Let us write $\hat{\phi}(\boldsymbol{k}, x_0)$ as the sum of two terms

$$\hat{\phi}(\boldsymbol{k}, x_0) = \hat{\phi}_+(\boldsymbol{k})e^{i\omega(\boldsymbol{k})x_0} + \hat{\phi}_-(\boldsymbol{k})e^{-i\omega(\boldsymbol{k})x_0} \tag{4.54}$$

The operators $\hat{\phi}_+(\boldsymbol{k})$ and $\hat{\phi}_+^\dagger(\boldsymbol{k})$ are not independent since the reality condition of the field $\hat{\phi}(\boldsymbol{x}, x_0)$ implies that

$$\hat{\phi}_+(\boldsymbol{k}) = \hat{\phi}_-^\dagger(-\boldsymbol{k}) \qquad \hat{\phi}_+^\dagger(\boldsymbol{k}) = \hat{\phi}_-(-\boldsymbol{k}) \tag{4.55}$$

This expansion is a solution of the equation of motion, the Klein-Gordon equation, provided $\omega(\boldsymbol{k})$ is given by

$$\omega(\boldsymbol{k}) = \sqrt{\boldsymbol{k}^2 + m^2} \tag{4.56}$$

Let us define the operator $\hat{a}(\boldsymbol{k})$ and its adjoint $\hat{a}^\dagger(\boldsymbol{k})$ by

$$\hat{a}(\boldsymbol{k}) = 2\omega(\boldsymbol{k})\hat{\phi}_-(\boldsymbol{k}) \qquad \hat{a}^\dagger(\boldsymbol{k}) = 2\omega(\boldsymbol{k})\hat{\phi}_-^\dagger(\boldsymbol{k}) \tag{4.57}$$

The operators $\hat{a}^\dagger(\boldsymbol{k})$ and $\hat{a}(\boldsymbol{k})$ obey the (generalized) creation-annihilation operator algebra

$$[\hat{a}(\boldsymbol{k}), \hat{a}^\dagger(\boldsymbol{k}')] = (2\pi)^3 2\omega(\boldsymbol{k})\, \delta^3(\boldsymbol{k} - \boldsymbol{k}') \tag{4.58}$$

In terms of the operators $\hat{a}^\dagger(\boldsymbol{k})$ and $\hat{a}(\boldsymbol{k})$ field operator becomes

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \left[\hat{a}(\boldsymbol{k}) e^{-i\omega(\boldsymbol{k})x_0 + i\boldsymbol{k}\cdot\boldsymbol{x}} + \hat{a}^\dagger(\boldsymbol{k}) e^{i\omega(\boldsymbol{k})x_0 - i\boldsymbol{k}\cdot\boldsymbol{x}}\right] \tag{4.59}$$

where we have chosen to normalize the operators in such a way that the phase space factor takes the Lorentz-invariant form $\dfrac{d^3k}{2\omega(\boldsymbol{k})}$.

The canonical momentum can also be expanded in a similar way

$$\widehat{\Pi}(x) = -i \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \omega(k) \Big[\hat{a}(\boldsymbol{k}) e^{-i\omega(\boldsymbol{k})x_0 + i\boldsymbol{k}\cdot\boldsymbol{x}} - \hat{a}^\dagger(\boldsymbol{k}) e^{i\omega(\boldsymbol{k})} e^{i\omega(\boldsymbol{k})x_0 - i\boldsymbol{k}\cdot\boldsymbol{x}}\Big] \tag{4.60}$$

Notice that, in both expansions, there are terms with positive and negative frequency, and that the terms with *positive frequency* have *creation* operators $\hat{a}^\dagger(\boldsymbol{k})$ while the terms with negative *frequency* have *annihilation* operators $\hat{a}(\boldsymbol{k})$. This observation motivates the notation

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \tag{4.61}$$

where the expansion of $\hat{\phi}_+$ has only positive frequency terms and the expansion of $\hat{\phi}_-$ has only negative frequency terms. This decomposition will turn out to be very useful.

4.3.2 The Hamiltonian and its spectrum

We will now write the Hamiltonian in terms of the operators $\hat{a}(\boldsymbol{k})$ and $\hat{a}^\dagger(\boldsymbol{k})$. The result is

$$\widehat{H} = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \frac{1}{2}\omega(\boldsymbol{k}) \left(\hat{a}(\boldsymbol{k})\hat{a}^\dagger(\boldsymbol{k}) + \hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k})\right) \tag{4.62}$$

This Hamiltonian needs to be normal-ordered relative to a ground state which we will now define.

A: Vacuum state

Let $|0\rangle$ be the state that is annihilated by all the operators $\hat{a}(\boldsymbol{k})$,

$$\hat{a}(\boldsymbol{k})|0\rangle = 0 \tag{4.63}$$

Relative to this state, which we will call the *vacuum* state, the Hamiltonian can be written on the form

$$\widehat{H} =: \widehat{H} : + E_0 \tag{4.64}$$

where $:\widehat{H}:$ is normal ordered relative to the state $|0\rangle$. In other words, in $:\widehat{H}:$ all the destruction operators appear the right of all the creation operators. Therefore the normal-ordered operator $:\widehat{H}:$ annihilates the vacuum state

$$:\widehat{H}: |0\rangle = 0 \tag{4.65}$$

The real number E_0 is the ground state energy. In this case it is equal to

$$E_0 = \int d^3k \frac{1}{2}\omega(\boldsymbol{k})\, \delta(0) \tag{4.66}$$

when $\delta(0)$, the delta function at zero momentum, is the infrared divergent quantity

$$\delta(0) = \lim_{p\to 0} \delta^3(\boldsymbol{p}) = \lim_{p\to 0} \int \frac{d^3x}{(2\pi)^3}\, e^{i\boldsymbol{p}\cdot\boldsymbol{x}} = \frac{V}{(2\pi)^3} \tag{4.67}$$

where V is the (infinite) volume of *space*. Thus, E_0 is extensive and can be written as $E_0 = \varepsilon_0 V$, where ε_0 is the ground state energy density. We find

$$\varepsilon_0 = \int \frac{d^3k}{(2\pi)^3} \frac{\omega(\boldsymbol{k})}{2} \equiv \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \sqrt{\boldsymbol{k}^2 + m^2} \tag{4.68}$$

Eq. (4.68) is the sum of the zero-point energies of all the oscillators. This quantity is formally divergent since the integral is dominated by the contributions with large momentum or, what is the same, short distances. This is an *ultraviolet divergence*. It is divergent because the system has an infinite number of degrees of freedom even in a finite volume. We will encounter other examples of similar divergencies in field theory. It is important to keep in mind that they are not artifacts of our scheme but that they result from the fact that the system is in continuous space-time and has an infinite number of degrees of freedom.

We can take two different points of view with respect to this problem. One possibility is simply to say that the ground state energy is not a physically observable quantity since any experiment will only yield information on excitation energies and, in this theory, they are finite. Thus, we may simply redefine the zero of the energy by dropping this term off. Normal ordering is then just the mathematical statement that all energies are measured relative to that of the ground state. As far as free field theory is concerned, this *subtraction* is sufficient since it makes the theory finite without affecting any physically observable quantity.

However, once interactions are considered, divergencies will show up in the formal computation of physical quantities. This procedure then requires further subtractions. An alternative approach consists in introducing a regulator or cutoff. The theory is now finite but one is left with the task of proving that the physics is independent of the cutoff procedure. This is the program of the Renormalization group. Although it is not presently known if there should be a fundamental cutoff in these theories, i.e. if there is a more fundamental description of Nature at short distances and high energies, such as it is postulated by String Theory, it is clear that if quantum field theories are to be regarded as effective *hydrodynamic* theories valid below some high energy scale, then a cutoff is actually natural.

B: Hilbert space

We can construct the spectrum of states by inspecting the normal-ordered Hamiltonian

$$:\widehat{H}:= \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})}\, \omega(\boldsymbol{k})\, \hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) \tag{4.69}$$

This Hamiltonian *commutes* with the *linear momentum* $\widehat{\boldsymbol{P}}$

$$\widehat{\boldsymbol{P}} = \int_{x_0 \text{ fixed}} d^3x\, \widehat{\Pi}(\boldsymbol{x}, x_0) \nabla \hat{\phi}(\boldsymbol{x}, x_0) \tag{4.70}$$

which, up to operator ordering ambiguities, is the quantum mechanical version of the classical linear momentum $\boldsymbol{P}$,

$$\boldsymbol{P} = \int_{x_0} d^3x\, T^{0j} \equiv \int_{x_0} d^3x\, \Pi(\boldsymbol{x}, x_0) \nabla \phi(\boldsymbol{x}, x_0) \tag{4.71}$$

In Fourier space $\widehat{\boldsymbol{P}}$ becomes

$$\widehat{\boldsymbol{P}} = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \boldsymbol{k}\, \hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) \tag{4.72}$$

The normal-ordered Hamiltonian $:\hat{H}:$ also commutes with the occupation numbers of the oscillators, $\hat{n}(\boldsymbol{k})$, defined by

$$\hat{n}(\boldsymbol{k}) \equiv \hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) \tag{4.73}$$

Since $\{\hat{n}(\boldsymbol{k})\}$ and the Hamiltonian $\hat{H}$ commute with each other, we can use a complete set of eigenstates of $\{\hat{n}(\boldsymbol{k})\}$ to span the Hilbert space. We will regard the excitations counted by $\hat{n}(k)$ as *particles* that have energy and momentum (in more general theories they will also have other quantum numbers). Their Hilbert space has an indefinite number of particles and it is called *Fock space*. The states $\{|\{n(\boldsymbol{k})\}\rangle\}$ of the Fock space, defined by

$$|\{n(\boldsymbol{k}\}\rangle = \prod_{\boldsymbol{k}} \mathcal{N}(\boldsymbol{k})[\hat{a}^\dagger(\boldsymbol{k})]^{n(\boldsymbol{k})}|0\rangle, \tag{4.74}$$

with $\mathcal{N}(\boldsymbol{k})$ being normalization constants, are eigenstates of the operator $\hat{n}(\boldsymbol{k})$

$$\hat{n}(\boldsymbol{k})|\{n(\boldsymbol{k})\}\rangle = (2\pi)^3 2\omega(\boldsymbol{k})n(\boldsymbol{k})|\{n(\boldsymbol{k})\rangle \tag{4.75}$$

These states span the *occupation number basis* of the Fock space.

The *total number operator* $\widehat{N}$

$$\widehat{N} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \hat{n}(\boldsymbol{k}) \tag{4.76}$$

commutes with the Hamiltonian $\widehat{H}$ and it is diagonal in this basis i.e.

$$\widehat{N}|\{n(\boldsymbol{k})\}\rangle = \int d^3k\; n(\boldsymbol{k})\; |\{n(\boldsymbol{k})\}\rangle \tag{4.77}$$

The energy of these states is

$$\widehat{H}|\{n(\boldsymbol{k})\}\rangle = \left[\int d^3k\; n(\boldsymbol{k})\omega(\boldsymbol{k}) + E_0\right] |\{n(\boldsymbol{k})\}\rangle \tag{4.78}$$

Thus, the *excitation energy* $\varepsilon(\{n(\boldsymbol{k})\})$ of this state is

$$\varepsilon(\boldsymbol{k}) = \int d^3k\; n(\boldsymbol{k})\omega(\boldsymbol{k}). \tag{4.79}$$

The total linear momentum operator $\widehat{\boldsymbol{P}}$ has an operator ordering ambiguity. It will be fixed by requiring that the vacuum state $|0\rangle$ be translationally invariant, i.e.

$$\widehat{\boldsymbol{P}}|0\rangle = 0. \tag{4.80}$$

In terms of creation and annihilation operators the total momentum operator is

$$\widehat{\boldsymbol{P}} = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \boldsymbol{k}\, \hat{n}(\boldsymbol{k}) \tag{4.81}$$

Thus, $\widehat{\boldsymbol{P}}$ is diagonal in the basis $|\{n(\boldsymbol{k})\}\rangle$ since

$$\widehat{\boldsymbol{P}}|\{n(\boldsymbol{k})\}\rangle = \left[\int d^3k\, \boldsymbol{k}\, n(\boldsymbol{k})\right] |\{n(\boldsymbol{k})\}\rangle \tag{4.82}$$

The state with lowest energy, the vacuum state $|0\rangle$ has $n(\boldsymbol{k}) = 0$, for all $\boldsymbol{k}$. Thus the vacuum state has zero momentum and it is translationally invariant.

The states $|\boldsymbol{k}\rangle$, defined by

$$|\boldsymbol{k}\rangle \equiv \hat{a}^\dagger(\boldsymbol{k})|0\rangle \tag{4.83}$$

have *excitation energy* $\omega(\boldsymbol{k})$ and total *linear momentum* $\boldsymbol{k}$. Thus, the states $\{|\boldsymbol{k}\rangle\}$ are particle-like excitations which have an energy dispersion curve

$$E = \sqrt{\boldsymbol{k}^2 + m^2}, \tag{4.84}$$

characteristic of a relativistic *particle* of momentum $\boldsymbol{k}$ and mass m. Thus, the excitations of the ground state of this *field theory* are particle-like, and have positive energy (relative to the vacuum state). From our discussion we can see that these *particles* are free since their energies and momenta are additive.

4.3.3 Causality

The starting point of the quantization procedure was to impose equal-time commutation relations among the canonical fields $\hat{\phi}(x)$ and their canonical momenta $\widehat{\Pi}(x)$. In particular, two field operators on different spatial locations *commute* at equal times. But, do they commute at different times?

To address this question let us calculate the commutator $\Delta(x - y)$

$$i\Delta(x - y) = [\hat{\phi}(x), \hat{\phi}(y)] \tag{4.85}$$

where $\hat{\phi}(x)$ and $\hat{\phi}(y)$ are Heisenberg field operators for *space-time* points x

and y respectively. From the Fourier expansion of the fields, we know that the field operator can be split into a sum of two terms

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \tag{4.86}$$

where $\hat{\phi}_+$ contains only creation operators and positive frequencies, and $\hat{\phi}_-$ contains only annihilation operators and negative frequencies. Thus the commutator is

$$\begin{aligned} i\Delta(x-y) =& [\hat{\phi}_+(x), \hat{\phi}_+(y)] + [\hat{\phi}_-(x), \hat{\phi}_-(y)] \\ &+ [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] \end{aligned} \tag{4.87}$$

The first two terms always vanish since the $\hat{\phi}_+$ operators commute among themselves and so do the operators $\hat{\phi}_-$. Thus, the only non-vanishing contributions are

$$\begin{aligned} i\Delta(x-y) =& [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] \\ =& \int d\bar{k} \int d\bar{k}' \Big\{ [\hat{a}^\dagger(\boldsymbol{k}), \hat{a}(\boldsymbol{k}')] \ \exp\Big(-i\omega(k)x_0 + i\boldsymbol{k}\cdot\boldsymbol{x} + i\omega(k')y_0 - i\boldsymbol{k}'\cdot\boldsymbol{y}\Big) \\ &+ [\hat{a}(\boldsymbol{k}), \hat{a}^\dagger(\boldsymbol{k}')] \exp\Big(i\omega(k)x_0 - i\boldsymbol{k}\cdot\boldsymbol{x} - i\omega(k'), y_0 + i\boldsymbol{k}'\cdot\boldsymbol{y}\Big)\Big\} \end{aligned} \tag{4.88}$$

where

$$\int d\bar{k} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \tag{4.89}$$

Furthermore, using the commutation relations of the creation and annihilation operators we find that the operator $\Delta(x-y)$ is proportional to the identity operator, and hence, it is actually a function. It is given by

$$i\Delta(x-y) = \int d\bar{k} \ \Big[e^{i\omega(\boldsymbol{k})(x_0-y_0)-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} - e^{-i\omega(\boldsymbol{k})(x_0-y_0)+i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}\Big] \tag{4.90}$$

With the help of the Lorentz-invariant function $\epsilon(k^0)$, defined by

$$\epsilon(k^0) = \frac{k^0}{|k^0|} \equiv \text{sign}(k^0) \tag{4.91}$$

we can write $\Delta(x-y)$ in the manifestly Lorentz invariant form

$$i\Delta(x-y) = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 - m^2)\epsilon(k^0) e^{-ik\cdot(x-y)} \tag{4.92}$$

The integrand of Eq.(4.92) vanishes unless the *mass shell condition*

$$k^2 - m^2 = 0 \tag{4.93}$$

is satisfied.

Notice that $\Delta(x-y)$ satisfies the initial condition

$$\partial_0 \Delta|_{x_0=y_0} = -\delta^3(\boldsymbol{x}-\boldsymbol{y}) \tag{4.94}$$

At equal times $x_0 = y_0$ the commutator vanishes,

$$\Delta(\boldsymbol{x}-\boldsymbol{y},0) = 0 \tag{4.95}$$

Furthermore, by Lorentz invariance, $\Delta(x-y)$ also vanishes if the space-time points x and y are separated by a *space-like* interval, $(x-y)^2 < 0$. This must be the case since $\Delta(x-y)$ is manifestly Lorentz invariant. Thus if it vanishes at equal times, where $(x-y)^2 = (x_0-y_0)^2 - (\boldsymbol{x}-\boldsymbol{y})^2 = -(\boldsymbol{x}-\boldsymbol{y}^2)^2 < 0$, it must vanish for all events with the negative values of $(x-y)^2$. This implies that, for events x and y which *are not* causally connected $\Delta(x-y) = 0$, and that $\Delta(x-y)$ is non-zero only for causally connected events, i.e. in the forward light-cone shown in Fig.4.1.

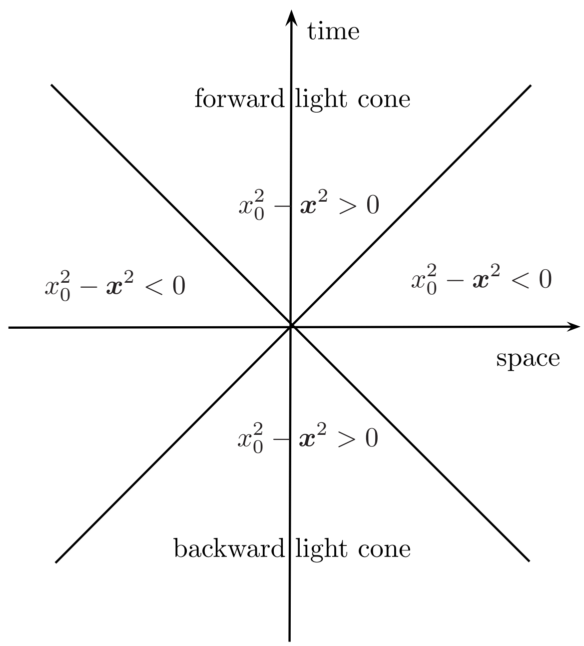

Figure 4.1 The Minkowski space-time.

4.4 Symmetries of the quantum theory

In our discussion of Classical Field Theory we discovered that the presence of continuous global symmetries implied the existence of constants of motion. In addition, the constants of motion were the generators of infinitesimal symmetry transformations. We will now see what role symmetries play in the quantized theory.

In the quantized theory all physical quantities are represented by operators that act on the Hilbert space of states. The classical statement that a quantity A is conserved if its Poisson Bracket with the Hamiltonian vanishes

$$\frac{dA}{dt} = \{A, H\}_{PB} = 0 \tag{4.96}$$

in the quantum theory becomes the operator identity

$$i\frac{d\widehat{A}_H}{dt} = [\widehat{A}_H, \widehat{H}] = 0 \tag{4.97}$$

we are are using the Heisenberg representation. Then, the constants of motion of the quantum theory are operators that commute with the Hamiltonian, $[\widehat{A}_H, \widehat{H}] = 0$.

Therefore, the quantum theory has a symmetry if and only if the charge $\widehat{Q}$, which is a hermitian operator associated with a classically conserved current $j^\mu(x)$ via the correspondence principle,

$$\widehat{Q} = \int_{x_0 \text{ fixed}} d^3x\, \hat{j}^0(\boldsymbol{x}, x_0) \tag{4.98}$$

is an operator that commutes with the Hamiltonian $\widehat{H}$

$$[\widehat{Q}, \widehat{H}] = 0 \tag{4.99}$$

If this is so, the charges $\widehat{Q}$ constitute a representation of the generators of the algebra of the Lie group of the symmetry transformations in the Hilbert space of the theory. The transformations $\widehat{U}(\alpha)$ associated with the symmetry

$$\widehat{U}(\alpha) = \exp(i\alpha\widehat{Q}) \tag{4.100}$$

are unitary transformations that act on the Hilbert space of the system.

For instance, we saw that for a translationally invariant system the classical energy-momentum four-vector P^μ

$$P^\mu = \int_{x_0} d^3x\, T^{0\mu} \tag{4.101}$$

is conserved. In the quantum theory P^0 becomes the Hamiltonian operator $\widehat{H}$, and P^i becomes the total momentum operator $\widehat{\boldsymbol{P}}$. In the case of a free scalar field, we saw before that these operators commute with each other, $[\widehat{\boldsymbol{P}}, \widehat{H}] = 0$. Thus, the eigenstates of the system have well defined total energy and total momentum. Since $\boldsymbol{P}$ is the generator of infinitesimal translations of the classical theory, it is easy to check that its equal-time Poisson Bracket with the field $\phi(x)$ is

$$\{\phi(\boldsymbol{x}, x_0), P^j\}_{PB} = \partial_x^j \phi \tag{4.102}$$

In the quantum theory the equivalent statement is that the field operator $\hat{\phi}(x)$ and the total momentum operator $\widehat{\boldsymbol{P}}$ satisfy the equal-time commutation relation

$$[\hat{\phi}(\boldsymbol{x}, x_0), \widehat{P}^j] = i\partial_x^j \hat{\phi}(\boldsymbol{x}, x_0) \tag{4.103}$$

Consequently, the field operators $\hat{\phi}(\boldsymbol{x} + \boldsymbol{a}, x_0)$ and $\hat{\phi}(\boldsymbol{x}, x_0)$ are related by

$$\hat{\phi}(\boldsymbol{x} + \boldsymbol{a}, x_0) = e^{i\boldsymbol{a}\cdot\widehat{\boldsymbol{P}}} \hat{\phi}(\boldsymbol{x}, x_0) e^{-i\boldsymbol{a}\cdot\widehat{\boldsymbol{P}}} \tag{4.104}$$

Translation invariance of the ground state $|0\rangle$ implies that it is a state with zero total momentum, $\widehat{\boldsymbol{P}}|0\rangle = 0$. For a finite displacement $\boldsymbol{a}$ we get

$$e^{i\boldsymbol{a}\cdot\widehat{\boldsymbol{P}}}|0\rangle = |0\rangle \tag{4.105}$$

which states that the state $|0\rangle$ is invariant under translations, and belongs to a one-dimensional representation of the group of global translations.

Let us discuss now what happens to *global* internal symmetries. The simplest case is the *free complex scalar field* $\phi(x)$ whose Lagrangian $\mathcal{L}$ is invariant under global phase transformations. If ϕ is a complex field, it can decomposed it into its real and imaginary parts

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \tag{4.106}$$

The classical Lagrangian for a free complex scalar field ϕ is

$$\mathcal{L} = \partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi \tag{4.107}$$

now splits into a sum of two independent terms

$$\mathcal{L}(\phi) = \mathcal{L}(\phi_1) + \mathcal{L}(\phi_2) \tag{4.108}$$

where $\mathcal{L}(\phi_1)$ and $\mathcal{L}(\phi_2)$ are the Lagrangians for the free scalar *real* fields ϕ_1 and ϕ_2. Likewise, the canonical momenta $\Pi(x)$ and $\Pi^*(x)$ are decomposed into

$$\Pi(x) = \frac{\delta \mathcal{L}}{\delta \partial_0 \phi} = \frac{1}{\sqrt{2}}(\dot{\phi}_1 - i\dot{\phi}_2) \qquad \Pi^*(x) = \frac{1}{\sqrt{2}}(\dot{\phi}_1 + i\dot{\phi}_2) \tag{4.109}$$

In the quantum theory the operators $\hat{\phi}$ and $\hat{\phi}^\dagger$ are no longer equal to each other, and neither are $\widehat{\Pi}$ and $\widehat{\Pi}^\dagger$. Still, the canonical quantization procedure tells us that $\hat{\phi}$ and $\widehat{\Pi}$ (and $\hat{\phi}^\dagger$ and $\widehat{\Pi}^\dagger$) satisfy the equal-time canonical commutation relations

$$[\hat{\phi}(\boldsymbol{x}, x_0), \widehat{\Pi}(\boldsymbol{y}, x_0)] = i\delta^3(\boldsymbol{x} - \boldsymbol{y}) \tag{4.110}$$

The theory of the free complex scalar field is solvable by the same methods that we used for a free real scalar field. Instead of a single creation annihilation algebra we must introduce now two algebras, with operators $\hat{a}_1(\boldsymbol{k})$ and $\hat{a}_1^\dagger(\boldsymbol{k})$, and $\hat{a}_2(\boldsymbol{k})$ and $\hat{a}_2^\dagger(\boldsymbol{k})$. Let $\hat{a}(\boldsymbol{k})$ and $\hat{b}(\boldsymbol{k})$ be defined by

$$\begin{aligned} \hat{a}(\boldsymbol{k}) &= \frac{1}{\sqrt{2}}\left(\hat{a}_1(\boldsymbol{k}) + i\hat{a}_2(\boldsymbol{k})\right), \quad \hat{a}^\dagger(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\left(\hat{a}_1^\dagger(\boldsymbol{k}) - i\hat{a}_2^\dagger(\boldsymbol{k})\right) \\ \hat{b}(\boldsymbol{k}) &= \frac{1}{\sqrt{2}}\left(\hat{a}_1(\boldsymbol{k}) - i\hat{a}_2(\boldsymbol{k})\right), \quad \hat{b}^\dagger(\boldsymbol{k}) = \frac{1}{\sqrt{2}}\left(\hat{a}_1^\dagger(\boldsymbol{k}) + i\hat{a}_2^\dagger(\boldsymbol{k})\right) \end{aligned} \tag{4.111}$$

which satisfy the algebra

$$[\hat{a}(\boldsymbol{k}), \hat{a}^\dagger(\boldsymbol{k}')] = [\hat{b}(\boldsymbol{k}), \hat{b}^\dagger(\boldsymbol{k}')] = (2\pi)^3 2\omega(\boldsymbol{k})\, \delta^3(\boldsymbol{k} - \boldsymbol{k}') \tag{4.112}$$

while all other commutators vanish.

The Fourier expansion for the fields now is

$$\begin{aligned} \hat{\phi}(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \left(\hat{a}(\boldsymbol{k}) e^{-ik\cdot x} + \hat{b}^\dagger(\boldsymbol{k}) e^{ik\cdot x}\right) \\ \hat{\phi}^\dagger(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \left(\hat{b}(k) e^{-ik\cdot x} + \hat{a}^\dagger(k) e^{ik\cdot x}\right) \end{aligned} \tag{4.113}$$

where $\omega(\boldsymbol{k}) = \sqrt{\boldsymbol{k}^2 + m^2}$ and $k_0 = \omega(\boldsymbol{k})$. In this notation, the normal-ordered Hamiltonian is

$$:\widehat{H}: = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})}\, \omega(\boldsymbol{k}) \left(\hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) + \hat{b}^\dagger(\boldsymbol{k})\hat{b}(\boldsymbol{k})\right) \tag{4.114}$$

The normal-ordered total linear momentum $\widehat{\boldsymbol{P}}$ is given by the similar expression

$$\widehat{\boldsymbol{P}} = \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})}\, \boldsymbol{k} \left(\hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) + \hat{b}^\dagger(\boldsymbol{k})\hat{b}(\boldsymbol{k})\right) \tag{4.115}$$

We see that there are two types of quanta, a and b. The field $\hat{\phi}$ creates b-quanta and it destroys a-quanta. The vacuum state has no quanta and is annihilated by both operators, $\hat{a}(\boldsymbol{k})|0\rangle = \hat{b}(\boldsymbol{k})|0\rangle = 0$. The one-particle states now have a two-fold degeneracy since the states $\hat{a}^\dagger(\boldsymbol{k})|0\rangle$ and $\hat{b}^\dagger(\boldsymbol{k})|0\rangle$ have one particle of type a and one of type b respectively. These states have exactly the same energy, $\omega(\boldsymbol{k})$, and the same momentum $\boldsymbol{k}$. Thus, for each value of the energy and of momentum, we have a two dimensional space of possible states. This degeneracy is a consequence of the symmetry: the states form multiplets.

What is the quantum operator that generates this symmetry? The classically conserved current is

$$j_\mu = i\phi^* \overset{\leftrightarrow}{\partial}_\mu \phi \tag{4.116}$$

In the quantum theory j_μ becomes the normal-ordered operator $:\hat{j}_\mu:$. The corresponding *global charge* $\widehat{Q}$ is

$$\begin{aligned}\widehat{Q} =& :\int d^3x \; i\left(\hat{\phi}^\dagger \partial_0 \hat{\phi} - (\partial_0 \hat{\phi}^\dagger)\hat{\phi}\right): \\ =& \int \frac{d^3k}{(2\pi)^3 2\omega(\boldsymbol{k})} \left(\hat{a}^\dagger(\boldsymbol{k})\hat{a}(\boldsymbol{k}) - \hat{b}^\dagger(\boldsymbol{k})\hat{b}(\boldsymbol{k})\right) \\ =& \hat{N}_a - \hat{N}_b \end{aligned} \tag{4.117}$$

where $\hat{N}_a$ and $\hat{N}_b$ are the number operators for quanta of type a and b respectively. Since $[\widehat{Q}, \widehat{H}] = 0$, the difference $\hat{N}_a - \hat{N}_b$ is conserved. Since this property is consequence of a symmetry, it is expected to hold in more general theories than the simple free-field case that we are discussing here, provided that $[\widehat{Q}, \widehat{H}] = 0$. Thus, although $\hat{N}_a$ and $\hat{N}_b$ in general may not be conserved *separately*, the difference $\hat{N}_a - \hat{N}_b$ will be conserved *if the symmetry is exact*.

Let us now briefly discuss how is this symmetry realized in the spectrum of states.

4.4.1 The vacuum state

The vacuum state has $N_a = N_b = 0$. Thus, the generator $\widehat{Q}$ annihilates the vacuum

$$\widehat{Q}|0\rangle = 0 \tag{4.118}$$

Therefore, the vacuum state is *invariant* (i.e. is a *singlet*) under the symmetry,

$$|0\rangle' = e^{i\widehat{Q}\alpha}|0\rangle = |0\rangle \tag{4.119}$$

Because the state $|0\rangle$ is always defined up to an overall phase factor, it spans a one-dimensional subspace of states which are invariant under the symmetry. This is the vacuum sector and, for this problem, is trivial.

4.4.2 One-particle states

There are two linearly-independent one-particle states, $|+,\boldsymbol{k}\rangle$ and $|-,\boldsymbol{k}\rangle$ defined by

$$|+,\boldsymbol{k}\rangle = \hat{a}^\dagger(\boldsymbol{k})\ |0\rangle \qquad |-,\boldsymbol{k}\rangle = \hat{b}^\dagger(\boldsymbol{k})\ |0\rangle \tag{4.120}$$

Both states have the same momentum $\boldsymbol{k}$ and energy $\omega(\boldsymbol{k})$. The $\widehat{Q}$-quantum numbers of these states, which we will refer to as their *charge*, are

$$\begin{aligned} \widehat{Q}|+,\boldsymbol{k}\rangle &= (\hat{N}_a - \hat{N}_b)\hat{a}^\dagger(\boldsymbol{k})|0\rangle = \hat{N}_a\ \hat{a}^\dagger(\boldsymbol{k})|0\rangle = +|+,\boldsymbol{k}\rangle \\ \widehat{Q}|-,\boldsymbol{k}\rangle &= (\hat{N}_a - \hat{N}_b)\ \hat{b}^\dagger(\boldsymbol{k})|0\rangle = -|-,\boldsymbol{k}\rangle \end{aligned} \tag{4.121}$$

Hence

$$\widehat{Q}|\sigma,\boldsymbol{k}\rangle = \sigma\ |\sigma,\boldsymbol{k}\rangle \tag{4.122}$$

where $\sigma = \pm 1$. Thus, the state $\hat{a}^\dagger(\boldsymbol{k})|0\rangle$ has *positive* charge while $\hat{b}^\dagger(\boldsymbol{k})|0\rangle$ has *negative* charge.

Under a finite transformation $\widehat{U}(\alpha) = \exp(i\alpha\widehat{Q})$ the states $|\pm,\boldsymbol{k}\rangle$ transform as follows

$$\begin{aligned} |+,\boldsymbol{k}\rangle' = \widehat{U}(\alpha)\ |+,\boldsymbol{k}\rangle &= \exp(i\alpha\hat{Q})\ |+,\boldsymbol{k}\rangle = e^{i\alpha}\ |+,\boldsymbol{k}\rangle \\ |-,\boldsymbol{k}\rangle' = \widehat{U}(\alpha)\ |-,\boldsymbol{k}\rangle &= \exp(i\alpha\hat{Q})|-,\boldsymbol{k}\rangle = e^{-i\alpha}\ |-,\boldsymbol{k}\rangle \end{aligned} \tag{4.123}$$

The field $\hat{\phi}(x)$ itself transforms as

$$\hat{\phi}'(x) = \exp(-i\alpha\widehat{Q})\ \hat{\phi}(x)\ \exp(i\alpha\widehat{Q}) = e^{i\alpha}\hat{\phi}(x) \tag{4.124}$$

since

$$[\widehat{Q},\hat{\phi}(x)] = -\hat{\phi}(x), \qquad [\widehat{Q},\hat{\phi}^\dagger(x)] = \hat{\phi}^\dagger(x) \tag{4.125}$$

Thus the one-particle states are doubly degenerate, and each state transforms non-trivially under the symmetry group.

By inspection of the Fourier expansion for the complex field $\hat{\phi}$, we see that $\hat{\phi}$ is a sum of two terms: a set of positive frequency terms, symbolized by $\hat{\phi}_+$, and a set of negative frequency terms, $\hat{\phi}_-$. In this case all *positive frequency terms create* particles of type b (which carry *negative* charge) while the *negative frequency terms annihilate* particles of type a (which carry *positive* charge). The states $|\pm, \boldsymbol{k}\rangle$ are commonly referred to as *particles* and *antiparticles*: particles have rest mass m, momentum $\boldsymbol{k}$ and charge $+1$ while the antiparticles have the same mass and momentum but carry charge -1. This charge is measured in units of the electromagnetic charge $-e$ (see the previous discussion on the gauge current).

We finally note that this theory contains an additional operator, the charge conjugation operator $\widehat{C}$, which maps particles into antiparticles and vice versa. This operator commutes with the Hamiltonian, $[\widehat{C}, \widehat{H}] = 0$. This property insures that the *spectrum* is invariant under charge conjugation. In other words, for every state of charge Q there exists a state with charge $-Q$, all other quantum numbers being the same.

Our analysis of the free complex scalar field can be easily extended to systems which are invariant under a more general symmetry group G. In all cases the classically conserved charges become operators of the quantum theory. Thus, there are as many charge operators $\widehat{Q}^a$ as generators are in the group. The charge operators represent the generators of the group in the Hilbert (or Fock) space of the system. The charge operators obey the same commutation relations as the generators themselves do. A simple generalization of the arguments that we have used here tells us that the states of the spectrum of the theory must transform under the irreducible representations of the symmetry group.

However, there is one important caveat that should be made. Our discussion of the *free* complex scalar field shows us that, in that case, the ground state is *invariant* under the symmetry. In general, the only possible invariant state is the *singlet state*. All other states are not invariant and transform non-trivially.

But, should the ground state always be invariant? In elementary quantum mechanics there is a theorem, due to Wigner and Weyl, which states that for a *finite system*, the ground state is always a singlet under the action of the symmetry group. However, there are many systems in Nature, such as magnets, Higgs phases, superconductors, and many others, which have ground states which are not invariant under the symmetries of the Hamiltonian. This phenomenon, known as *spontaneous symmetry breaking*, does not occur in simple *free* field theories but it does happen in interacting field theories. We will return to this important question in chapter 12.