

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 :

$$p = \frac{\partial L}{\partial \dot{q}} \quad (4.1)$$

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

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

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

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \dot{q} = \frac{\partial H}{\partial p} \quad (4.3)$$

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

$$\{q, p\}_{PB} = 1 \quad \{q, q\}_{PB} = \{p, p\}_{PB} = 0 \quad (4.4)$$

where

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

In Quantum Mechanics, the primitive (or fundamental) notion is the concept of a *physical state*. A physical state of a system is represented by a *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 linear, 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 $|\Phi\rangle \in \mathcal{H}$,

$$\hat{A}|\Psi\rangle = |\Phi\rangle \quad (4.6)$$

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 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} ,

$$|\Psi\rangle = \sum_{\lambda} \Psi_{\lambda} |\lambda\rangle \quad (4.7)$$

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,

$$\langle\lambda|\mu\rangle = \delta_{\lambda\mu} \quad (4.8)$$

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

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1 \quad (4.9)$$

the action of the operator \hat{A} on the state $|\Psi\rangle$ is proportional to the state $|\Phi\rangle$

$$\hat{A}|\Psi\rangle = \alpha|\Phi\rangle \quad (4.10)$$

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

$$\alpha = \langle\Phi|\hat{A}|\Psi\rangle \quad (4.11)$$

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, $\hbar \rightarrow 0$, the operators should effectively become numbers, *i. e.* they commute 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} , both of which act on the Hilbert space of states \mathcal{H} , and are *required* to obey the *canonical commutation relations*

$$[\hat{q}, \hat{p}] = i\hbar \quad [\hat{q}, \hat{q}] = [\hat{p}, \hat{p}] = 0 \quad (4.12)$$

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

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (4.13)$$

In particular, two operators that do not commute with each other cannot be diagonalized simultaneously. Hence it is not possible to measure simultaneously two non-commuting observables with arbitrary precision in the same physical state. 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* $\hat{H}(\hat{q}, \hat{p})$ which is obtained by replacing the dynamical variables with the corresponding operators. Other classical dynamical quantities in Quantum Mechanics are similarly associated with quantum operators that act on the Hilbert space of states. 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}

$$\langle\Psi|\hat{A}^\dagger|\Phi\rangle \equiv \langle\Phi|\hat{A}\Psi\rangle^* \quad (4.14)$$

and \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

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

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.*,

$$\hat{q}|q\rangle = q|q\rangle \quad (4.16)$$

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

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

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

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

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

$$\Psi(q) = \langle q|\Psi\rangle, \quad (4.19)$$

the amplitude to find the system at coordinate q in this state, are the values of the *wave function* associated with 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. In fact, just as in Classical Mechanics, 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

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

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

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

Hence, we can write

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

Thus,

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

We can now use this property to compute the matrix element

$$\langle q|\exp\left(\frac{i}{\hbar}a\hat{p}\right)|\Psi\rangle \equiv \Psi(q+a) \quad (4.24)$$

For a infinitesimally small, it can be approximated by

$$\Psi(q+a) \approx \Psi(q) + \frac{i}{\hbar}a\langle q|\hat{p}|\Psi\rangle + \dots \quad (4.25)$$

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

$$\langle q|\hat{p}|\Psi\rangle = \frac{\hbar}{i} \lim_{a \rightarrow 0} \frac{\Psi(q+a) - \Psi(q)}{a} \quad (4.26)$$

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

$$\langle q|\hat{p}|\Psi\rangle \equiv \frac{\hbar}{i} \frac{\partial}{\partial q} \Psi(q) = \frac{\hbar}{i} \frac{\partial}{\partial q} \langle q|\Psi\rangle \quad (4.27)$$

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

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial q} \quad (4.28)$$

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,

$$\Pi(x) = \frac{\partial \mathcal{L}}{\delta \partial_0 \phi(x)} \quad (4.29)$$

On a given time surface x_0 , the classical Hamiltonian is

$$H = \int d^3x [\Pi(\mathbf{x}, x_0)\partial_0\phi(\mathbf{x}, x_0) - \mathcal{L}(\phi, \partial_\mu\phi)] \quad (4.30)$$

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

$$[\hat{\phi}(\mathbf{x}), \hat{\Pi}(\mathbf{y})] = i\hbar\delta(\mathbf{x} - \mathbf{y}) \quad (4.31)$$

In the *field representation*, the Hilbert space is the vector space of wave functions Ψ which are *functionals* of the field configurations $\{\phi(\mathbf{x})\}$,

$$\Psi[\{\phi(\mathbf{x})\}] \equiv \langle \{\phi(\mathbf{x})\} | \Psi \rangle \quad (4.32)$$

In this representation, the field is a diagonal operator

$$\langle \{\phi\} | \hat{\phi}(\mathbf{x}) | \Psi \rangle \equiv \phi(\mathbf{x}) \langle \{\phi(\mathbf{x})\} | \Psi \rangle = \phi(\mathbf{x}) \Psi[\{\phi\}] \quad (4.33)$$

The canonical momentum $\hat{\Pi}(\mathbf{x})$ is not diagonal in this representation but it acts like a functional differential operator,

$$\langle \{\phi\} | \hat{\Pi}(\mathbf{x}) | \Psi \rangle \equiv \frac{\hbar}{i} \frac{\delta}{\delta\phi(\mathbf{x})} \Psi[\{\phi\}] \quad (4.34)$$

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

$$i\hbar\partial_0\Psi[\{\phi\}, x_0] = \hat{H}\Psi[\{\phi\}, x_0] \quad (4.35)$$

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

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 - V(\phi) \quad (4.36)$$

the quantum mechanical Hamiltonian operator \hat{H} is

$$\hat{H} = \int d^3x \left\{ \frac{1}{2}\hat{\Pi}^2(\mathbf{x}) + \frac{1}{2}(\nabla\hat{\phi}(\mathbf{x}))^2 + V(\phi(\mathbf{x})) \right\} \quad (4.37)$$

The stationary states are the eigenstates of the Hamiltonian \hat{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 an alternative approach has been devised. This is the *Heisenberg Picture*.

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

$$\hat{A}_H(x_0) = e^{\frac{i}{\hbar}\hat{H}x_0} \hat{A} e^{-\frac{i}{\hbar}\hat{H}x_0} \quad (4.38)$$

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

$$i\hbar\partial_0\hat{A}_H(x_0) = [\hat{A}_H(x_0), \hat{H}] \quad (4.39)$$

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

$$\partial_0 A(x_0) = \{A(x_0), H\}_{PB} \quad (4.40)$$

where it is assumed that all the time dependence in A comes from the time dependence of the coordinates and momenta.

In the Heisenberg picture both $\hat{\phi}(\mathbf{x}, x_0)$ and $\hat{\Pi}(\mathbf{x}, x_0)$ are time dependent operators which obey the equations of motion

$$i\hbar\partial_0\hat{\phi}(\mathbf{x}, x_0) = [\hat{\phi}(\mathbf{x}, x_0), \hat{H}], \quad i\hbar\partial_0\hat{\Pi}(\mathbf{x}, x_0) = [\hat{\Pi}(\mathbf{x}, x_0), \hat{H}] \quad (4.41)$$

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

$$[\hat{\phi}(\mathbf{x}, x_0), \hat{\Pi}(\mathbf{y}, x_0)] = i\hbar\delta(\mathbf{x} - \mathbf{y}) \quad (4.42)$$

4.3 Quantized elastic waves in a solid: Phonons

Let us consider the problem of the quantum dynamics of a linear array of atoms (shown in Fig.4.1). We will see below that this problem is closely related to the problem of quantization of a free scalar field. We will consider the simple case of a one-dimensional array of atoms, a chain. Each atom has mass M and their classical equilibrium positions are the regularly spaced lattice sites $x_n^0 = na$, ($n = 1, \dots, N$) where a is the lattice spacing. I will assume that we have a system with N atoms and, therefore that the length L of the chain is $L = Na$. To simplify matters, I will assume that the chain is actually a ring and, thus, the $N + 1$ -th atom is the same as the

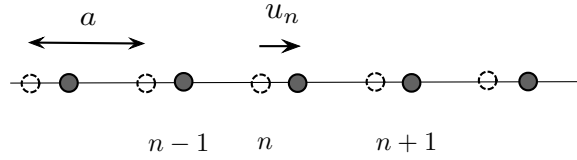


Figure 4.1 A model of an elastic one-dimensional solid.

1st atom. The dynamics of this system can be specified in terms of a set of coordinates $\{u_n\}$ which represent the position of each atom *relative* to their classical equilibrium positions x_n^0 *i.e.*, the actual position x_n of the n^{th} atom is $x_n = x_n^0 + u_n$.

The Lagrangian of the system is a function of the coordinates $\{u_n\}$, the displacements, and of their time derivatives $\{\dot{u}_n\}$. In general the Lagrangian L it will be the difference of the kinetic energy of the atoms minus their potential energy, *i.e.*,

$$L(\{u_n\}, \{\dot{u}_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{M}{2} \left(\frac{du_n}{dt} \right)^2 - V(\{u_n\}) \quad (4.43)$$

We will be interested in the study of the small oscillations of the system. Thus, the potential will have a minimum at the classical equilibrium positions $\{u_n = 0\}$ (which we will assume to be unique). For small oscillations $V(\{u_n\})$ can be expanded in powers

$$V(\{u_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\frac{D}{2} (u_{n+1} - u_n)^2 + \frac{K}{2} u_n^2 + \dots \right] \quad (4.44)$$

Here D is an elastic constant (*i.e.*, spring constant!) which represents the restoring forces that keep the crystal together. The constant K is a measure of the strength of an external potential which favors the placement of the atoms at their classical equilibrium positions. For an isolated system, $K = 0$ but $D \neq 0$. This must be the case since an isolated system must be translationally invariant and, therefore, V must not change under a constant, uniform, displacement of all the atoms by some amount a , $u_n \rightarrow u_n + a$. The term proportional to u_n^2 breaks this symmetry of uniform continuous displacements, although it does not spoil the discrete symmetry $n \rightarrow n + m$.

Let us now proceed to study the quantum mechanics of this system. Each atom has a coordinate $u_n(t)$ and a canonical momentum $p_n(t)$ which is

defined in the usual way

$$p_n(t) = \frac{\partial L}{\partial \dot{u}_n(T)} = M\dot{u}_n(t) \quad (4.45)$$

The quantum Hamiltonian for a chain with an even number of sites N is

$$H(\{\hat{u}_n\}, \{\hat{p}_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\frac{\hat{p}_n^2}{2M} + \frac{D}{2}(\hat{u}_{n+1} - \hat{u}_n)^2 + \frac{K}{2}\hat{u}_n^2 + \dots \right] \quad (4.46)$$

where the coordinates and momenta obey the commutation relations

$$[\hat{u}_n, \hat{p}_m] = i\hbar\delta_{n,m}, \quad [\hat{u}_n, \hat{u}_m] = [\hat{p}_n, \hat{p}_m] = 0. \quad (4.47)$$

For this simple system, the Hilbert space can be identified with the tensor product of the Hilbert spaces of each individual atom. Thus, if $|\Psi\rangle_n$ denotes an arbitrary state in the Hilbert space of the n th atom, the states of the chain $|\Psi\rangle$ can be written in the form

$$|\Psi\rangle = |\Psi\rangle_1 \otimes \dots \otimes |\Psi\rangle_n \otimes \dots \otimes |\Psi\rangle_N \equiv |\Psi_1, \dots, \Psi_N\rangle \quad (4.48)$$

For instance, a set of basis states can be constructed by using the coordinate representation. Thus, if the state $|u_n\rangle$ is an eigenstate of \hat{u}_n with eigenvalue u_n

$$\hat{u}_n|u_n\rangle = u_n|u_n\rangle \quad (4.49)$$

we can write a set of basis states

$$|u_1, \dots, u_N\rangle \quad (4.50)$$

of the form

$$|u_1, \dots, u_N\rangle = |u_1\rangle \otimes \dots \otimes |u_N\rangle \quad (4.51)$$

In this basis, the wave functions are

$$\Psi(u_1, \dots, u_N) = \langle u_1, \dots, u_N | \Psi \rangle \quad (4.52)$$

By inspecting the Hamiltonian it is easy to recognize that in this case it represents a set of N coupled harmonic oscillators. Since the system is periodic and invariant under lattice shifts $n \rightarrow n + m$ (m integer), it is natural to expand the coordinates \hat{u}_n in a Fourier series

$$\hat{u}_n = \frac{1}{N} \sum_k \tilde{u}_k e^{ikn} \quad (4.53)$$

where k is a label, that will be related with the lattice momentum, and \tilde{u}_k

are the Fourier components of \hat{u}_n . The fact that we have imposed periodic boundary conditions (PBC's), *i.e.*, that the chain is a ring, means that

$$\hat{u}_n = \hat{u}_{n+N} \quad (4.54)$$

This relation can hold only if the labels k satisfy

$$e^{ikN} = 1 \quad (4.55)$$

which restricts the values of k to the *discrete* set

$$k_m = 2\pi \frac{m}{N}, \quad m = -\frac{N}{2} + 1, \dots, \frac{N}{2} \quad (4.56)$$

where we have set the lattice spacing to unity, $a_0 = 1$. Thus the expansion of \hat{u}_n is

$$\hat{u}_n = \frac{1}{N} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \tilde{u}_{k_m} e^{ik_m n} \quad (4.57)$$

The spacing Δk between two consecutive values of the label k (k_m and k_{m+1}) is

$$\Delta k = k_{m+1} - k_m = \frac{2\pi}{N} \quad (4.58)$$

which vanishes in the thermodynamic limit, $N \rightarrow \infty$. In particular, the momentum label k_n runs over the range $(-\frac{N}{2} + 1)\frac{2\pi}{N} \leq k_m \leq \frac{N}{2}$. Thus, in the limit $N \rightarrow \infty$ the momenta fill up densely the real interval $(-\pi, \pi]$.

We then conclude that, in the thermodynamic limit, $N \rightarrow \infty$, the momentum sum converges to the integral

$$\hat{u}_n = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \tilde{u}_{k_m} e^{ik_m n} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \tilde{u}(k) e^{ikn} \quad (4.59)$$

Since \hat{u}_n is a real hermitian operator, the Fourier components $\tilde{u}(k)$ must satisfy

$$\tilde{u}^\dagger(k) = \tilde{u}(-k) \quad (4.60)$$

The Fourier component $\tilde{u}(k)$ can be written as a linear combination of operators \hat{u}_n of the form

$$\tilde{u}(k) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \hat{u}_n e^{-ikn} \quad (4.61)$$

where we used definition of the periodic Dirac delta function,

$$2\pi\delta_P(k-q) \equiv \sum_{m=-\infty}^{+\infty} 2\pi\delta(k-q+2\pi m) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{i(k-q)n} \quad (4.62)$$

which is defined in the thermodynamic limit.

The momentum operators \hat{p}_n can also be expanded in Fourier series. Their expansions are

$$\hat{p}_n = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \tilde{p}(k) e^{ikn}, \quad \tilde{p}(k) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-ikn} \hat{p}_n \quad (4.63)$$

and satisfy

$$\tilde{p}^\dagger(k) = \tilde{p}(-k) \quad (4.64)$$

The transformation $(\hat{u}_n, \hat{p}_n) \rightarrow (\tilde{u}(k), \tilde{p}(k))$ is a canonical transformation. Indeed, the Fourier amplitudes $\tilde{u}(k)$ and $\tilde{p}(k)$ obey the commutation relations

$$\begin{aligned} [\tilde{u}(k), \tilde{p}(k')] &= \sum_{n, n'=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-i(kn+k'n')} [\tilde{u}_n, \tilde{p}_{n'}] \\ &= i\hbar \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-i(k+k')n} \end{aligned} \quad (4.65)$$

Hence, in the thermodynamic limit we find

$$[\tilde{u}(k), \tilde{p}(k')] = i\hbar 2\pi \delta_P(k+k') \quad (4.66)$$

and

$$[\tilde{u}(k), \tilde{p}(k')] = [\tilde{p}(k), \tilde{p}(k')] = 0 \quad (4.67)$$

We can now write the Hamiltonian H in terms of the Fourier components $\tilde{u}(k)$ and $\tilde{p}(k)$. We find

$$H = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left[\frac{1}{2M} \tilde{p}^\dagger(k) \tilde{p}(k) + \frac{M}{2} \omega^2(k) \tilde{u}^\dagger(k) \tilde{u}(k) \right] \quad (4.68)$$

where $\omega^2(k)$ is

$$\omega^2(k) = \frac{K}{M} + \frac{4D}{M} \sin^2\left(\frac{k}{2}\right) \quad (4.69)$$

Thus, the system decouples into its normal modes. The frequency $\omega(k)$ is shown in Fig.4.2. It is instructive to study the long-wave length limit, $k \rightarrow 0$.

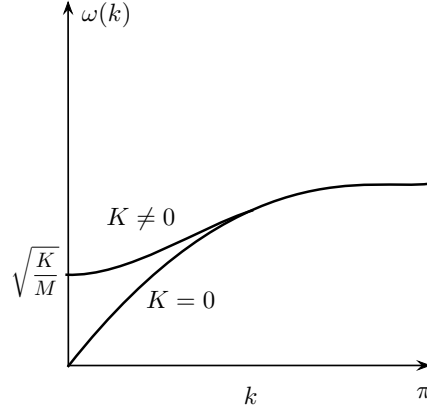


Figure 4.2 The dispersion relation $\omega(k)$.

For $K = 0$ *i.e.*, if there is no external potential, $\omega(k)$ vanishes linearly as $k \rightarrow 0$,

$$\omega(k) \approx \sqrt{\frac{D}{M}} |k| \quad (K = 0) \quad (4.70)$$

However, for non-zero K , again in the limit $k \rightarrow 0$, we find instead

$$\omega(k) \approx \sqrt{\frac{K}{M} + \frac{D}{M} k^2} \quad (4.71)$$

If we now restore a lattice constant $a_0 \neq 1$, $k = \tilde{k} a_0$ we can write $\omega(\tilde{k})$ in the form

$$\omega(\tilde{k}) = v_s \sqrt{\tilde{m}^2 v_s^2 + \tilde{k}^2} \quad (4.72)$$

where v_s is the speed of propagation of sound in the chain,

$$v_s = \sqrt{\frac{D}{M}} a_0 \equiv \sqrt{\frac{D a_0}{\bar{\rho}}} \quad (4.73)$$

where $\bar{\rho}$ is the (linear) density. The “mass” \tilde{m} is

$$\tilde{m} = \frac{\omega_0}{v_s^2} \quad (4.74)$$

where $\omega_0 = \sqrt{\frac{K}{M}}$. Thus, the waves that propagate on this chain behave as “relativistic” particles with mass \tilde{m} and a “speed of light” v_s . Indeed,

the long wavelength limit, $k \rightarrow 0$, the Lagrangian of the discrete chain, Eq.(4.43), can be written as an integral

$$L = a_0 \sum_n \frac{1}{2} \left(\frac{M}{a_0} \right) \left(\frac{\partial u_n}{\partial t} \right)^2 - \frac{a_0}{2} \sum_n D a_0 \left(\frac{u_{n+1} - u_n}{a_0} \right)^2 - \frac{a_0}{2} \sum_n \frac{K}{a_0} u_n^2 \quad (4.75)$$

Thus, as $a_0 \rightarrow 0$ and $N \rightarrow \infty$, with fixed total length $\ell = N a_0$, the sums converge to the integral

$$L = \bar{\rho} \int_{-\ell/2}^{\ell/2} dx \left\{ \frac{1}{2} \left(\frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} v_s^2 \left(\frac{\partial u}{\partial x} \right)^2 - \frac{1}{2} \bar{m}^2 v_s^4 u^2(x) \right\} \quad (4.76)$$

Aside from the overall factor of $\bar{\rho}$, the mass density, we see that the Lagrangian for the linear chain is, in the long wavelength limit (or *continuum limit*) the same as the Lagrangian for the Klein-Gordon field $u(x)$ in one-space dimension. The last term of this Lagrangian is precisely the mass term for the Lagrangian of the Klein-Gordon field. This explains the choice of the symbol \bar{m} . Indeed, upon the change of variables

$$x_0 = v_s t \quad x_1 = x \quad (4.77)$$

and by defining the rescaled field

$$\varphi = \sqrt{\bar{\rho} v_s} u \quad (4.78)$$

we see immediately that the Lagrangian density \mathcal{L} is

$$\mathcal{L} = \frac{1}{2} (\partial_0 \varphi)^2 - \frac{1}{2} (\partial_1 \varphi)^2 - \frac{1}{2} \bar{m}^2 v_s^4 \varphi^2 \quad (4.79)$$

This is the Lagrangian density of a free massive scalar field in 1 + 1 space-time dimension.

Returning to the quantum theory, we seek to find the eigenstates of the normal-mode Hamiltonian. Let $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ be the operators defined by

$$\begin{aligned} \hat{a}^\dagger(k) &= \frac{1}{\sqrt{2M\hbar\omega(k)}} \left(M\omega(k)\tilde{u}^\dagger(k) - i\tilde{p}^\dagger(k) \right) \\ \hat{a}(k) &= \frac{1}{\sqrt{2M\hbar\omega(k)}} \left(M\omega(k)\tilde{u}(k) + i\tilde{p}(k) \right) \end{aligned} \quad (4.80)$$

These operators satisfy the commutation relations

$$\begin{aligned} [\hat{a}(k), \hat{a}(k')] &= [\hat{a}^\dagger(k), \hat{a}^\dagger(k')] = 0 \\ [\hat{a}(k), \hat{a}^\dagger(k')] &= 2\pi\delta_P(k + k') \end{aligned} \quad (4.81)$$

Up to normalization constants, the operators $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ obey the algebra of creation and annihilation operators.

In terms of the creation and annihilation operators, the momentum space oscillator operators $\tilde{u}(k)$ and $\tilde{p}(k)$ are

$$\begin{aligned}\tilde{u}(k) &= \sqrt{\frac{\hbar}{2M\omega(k)}} \left(\hat{a}(k) + \hat{a}^\dagger(-k) \right) \\ \tilde{p}(k) &= \sqrt{2M\hbar\omega(k)} \frac{1}{2i} \left(\hat{a}(k) - \hat{a}^\dagger(-k) \right)\end{aligned}\quad (4.82)$$

Thus, the coordinate space operators \hat{u}_n and \hat{p}_n have the Fourier expansions

$$\begin{aligned}\hat{u}_n &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sqrt{\frac{\hbar}{2M\omega(k)}} \left(\hat{a}(k) e^{ikn} + \hat{a}^\dagger(k) e^{-ikn} \right) \\ \hat{p}_n &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sqrt{2M\hbar\omega(k)} \frac{1}{2i} \left(\hat{a}(k) e^{ikn} - \hat{a}^\dagger(k) e^{-ikn} \right)\end{aligned}\quad (4.83)$$

The normal-mode Hamiltonian has a very simple form in terms of the creation and annihilation operators

$$H = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} \left(\hat{a}^\dagger(k)\hat{a}(k) + \hat{a}(k)\hat{a}^\dagger(k) \right)\quad (4.84)$$

It is customary to write H in such a way that the creation operators always appear *to the left* of annihilation operators. This procedure is called *normal ordering*. Given an arbitrary operator \hat{A} , we will denote by $:\hat{A}:$ the *normal ordered operator*. We can see by inspection that \hat{H} can be written as a sum of two terms: a normal ordered operator $:\hat{H}:$ and a complex number. The complex number results from using the commutation relations. Indeed, by operating on the last term of the Hamiltonian of Eq.(4.84), we get

$$\hat{a}(k)\hat{a}^\dagger(k) = [\hat{a}(k), \hat{a}^\dagger(k)] + \hat{a}^\dagger(k)\hat{a}(k)\quad (4.85)$$

The commutator $[\hat{a}(k), \hat{a}^\dagger(k)]$ is the divergent quantity

$$\begin{aligned}[\hat{a}(k), \hat{a}^\dagger(k)] &= \lim_{k' \rightarrow k} 2\pi\delta_P(k - k') = \lim_{k' \rightarrow k} 2\pi \sum_{m=-\infty}^{+\infty} \delta(k - k' + 2\pi m) \\ &= \lim_{k' \rightarrow k} \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{i(k-k')n} = N\end{aligned}\quad (4.86)$$

which diverges in the thermodynamic limit, $N \rightarrow \infty$.

Using these results, we can write \hat{H} in the form

$$\hat{H} = : \hat{H} : + E_0 \quad (4.87)$$

where $: \hat{H} :$ is the normal-ordered Hamiltonian

$$: \hat{H} := \int_{-\pi}^{\pi} \frac{dk}{2\pi} \hbar\omega(k) \hat{a}^\dagger(k)\hat{a}(k) \quad (4.88)$$

and the real number E_0 is given by

$$E_0 = N \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} \quad (4.89)$$

We will see below that E_0 is the ground state energy of this system. The linear divergence of E_0 as $N \rightarrow \infty$ is natural since the ground state energy must be an *extensive* quantity, *i.e.*, it scales like the length (volume) of the chain (system). Notice that the integral in Eq.(4.89) runs over the finite momentum interval $(-\pi, \pi)$, *i.e.* the first Brillouin zone. In the next subsection we will encounter a similar result for the free relativistic scalar field but with an integral running over an unbounded momentum range, which will lead to an ultraviolet (UV) divergence of the ground state energy (among other quantities). Thus, in this simple chain system we have a cutoff at large momentum imposed by the discrete microscopic lattice. In this case there is no UV divergence but instead quantities such as the ground state energy have a high sensitivity to the value of the UV cutoff, the momentum scale $\frac{\pi}{a_0}$, where a_0 is the lattice spacing.

We are now ready to construct the spectrum of eigenstates of this system.

4.3.1 Ground state

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

$$\hat{a}(k)|0\rangle = 0 \quad (4.90)$$

This state is an eigenstate with eigenvalue E_0 since

$$\hat{H}|0\rangle = : \hat{H} : |0\rangle + E_0|0\rangle = E_0|0\rangle \quad (4.91)$$

where we have used the fact that $|0\rangle$ is annihilated by the normal-ordered Hamiltonian $: \hat{H} :$. This is the *ground state* of the system since the energy of all other states is higher. Thus, E_0 is the energy of the ground state. Notice that E_0 is the sum of the zero-point energy of all the oscillators.

The wave function for the ground state can be constructed quite easily. Let $\Psi_0(\{\hat{u}(k)\}) = \langle \{\hat{u}(k)\} | 0 \rangle$ be the wave function of the ground state. The

condition that $|0\rangle$ be annihilated by all the operators $\hat{a}(k)$ means that the matrix element $\langle\{\tilde{u}(k)\}|\hat{a}(k)|0\rangle$ has to vanish identically. The definition of $\hat{a}(k)$ yields the condition

$$0 = M\omega(k) \langle\{\tilde{u}(k)\}|\tilde{u}(k)|0\rangle + i\langle\{\tilde{u}(k)\}|\tilde{p}(k)|0\rangle \quad (4.92)$$

The commutation relation

$$[\tilde{u}(k), \tilde{p}(k')] = i\hbar 2\pi \delta_P(k + k') \quad (4.93)$$

implies that, in the coordinate representation $\tilde{p}(k)$ must be the functional differential operator

$$\langle\{\tilde{u}(k)|\tilde{p}(k)|0\rangle = \frac{\hbar}{i} 2\pi \frac{\delta}{\delta\tilde{u}(k)} \Psi_0(\{\hat{u}(k)\}) \quad (4.94)$$

Thus, the wave functional Ψ_0 must obey the differential equation

$$M\omega(k) \hat{u}^*(k) \Psi_0(\{\hat{u}(k)\}) + 2\pi\hbar \frac{\delta}{\delta\hat{u}(k)} \Psi_0(\{\hat{u}(k)\}) = 0 \quad (4.95)$$

for each value of $k \in [-\pi, \pi)$. Clearly Ψ_0 has the form of a product

$$\Psi_0(\{\hat{u}(k)\}) = \prod_k \Psi_{0,k}(\tilde{u}(k)) \quad (4.96)$$

where the wave function $\Psi_{0,k}(\tilde{u}(k))$ satisfies

$$M\omega(k) \tilde{u}^*(k) \Psi_{0,k}(u(k)) + 2\pi\hbar \frac{\partial}{\partial u(k)} \Psi_{0,k}(u(k)) = 0 \quad (4.97)$$

The solution of this equation is the ground state wave function for the k -th oscillator

$$\Psi_{0,k}(u(k)) = \mathcal{N}(k) \exp\left(-\frac{1}{2} \left(\frac{M\omega(k)}{2\pi\hbar}\right) |\tilde{u}|^2(k)\right) \quad (4.98)$$

where $\mathcal{N}(k)$ is a normalization factor. The total wave function for the ground state is

$$\Psi_0(\{\tilde{u}(k)\}) = \mathcal{N} \exp\left[-\frac{1}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(\frac{M\omega(k)}{2\pi\hbar}\right) |\tilde{u}|^2(k)\right] \quad (4.99)$$

where \mathcal{N} is another normalization constant. Notice that this wave function is a functional of the oscillator variables $\{\tilde{u}(k)\}$.

4.3.2 One-Particle States

Let the ket $|1_k\rangle$ denote the one-particle state

$$|1_k\rangle \equiv \hat{a}^\dagger(k)|0\rangle \quad (4.100)$$

This state is an eigenstate of \hat{H} with eigenvalue $E_1(k)$

$$\hat{H}|1_k\rangle =: \hat{H}: |1_k\rangle + E_0|1_k\rangle \quad (4.101)$$

The normal-ordered term now does give a contribution since

$$\begin{aligned} : \hat{H}: |1_k\rangle &= \left(\int_{-\pi}^{\pi} \frac{dk'}{2\pi} \hbar\omega(k') \hat{a}^\dagger(k')\hat{a}(k') \right) \hat{a}^\dagger(k)|0\rangle \\ &= \int_{-\pi}^{\pi} \frac{dk'}{2\pi} \hbar\omega(k') \left(\hat{a}^\dagger(k')[\hat{a}(k'), \hat{a}^\dagger(k)]|0\rangle + \hat{a}^\dagger(k')\hat{a}^\dagger(k)\hat{a}(k')|0\rangle \right) \end{aligned} \quad (4.102)$$

The result is

$$: \hat{H}: |1_k\rangle = \int_{-\pi}^{\pi} \frac{dk'}{2\pi} \hbar\omega(k') \hat{a}^\dagger(k') 2\pi\delta_P(k' - k) |0\rangle \quad (4.103)$$

since the last term vanishes. Hence

$$: \hat{H}: |1_k\rangle = \hbar\omega(k) \hat{a}^\dagger(k) |0\rangle \equiv \hbar\omega(k) |1_k\rangle \quad (4.104)$$

Therefore, we find

$$\hat{H}|1_k\rangle = (\hbar\omega(k) + E_0) |1_k\rangle \quad (4.105)$$

Let $\varepsilon(k)$ be the excitation energy

$$\varepsilon(k) \equiv E_1(k) - E_0(k) = \hbar\omega(k) \quad (4.106)$$

Thus the one-particle states represent quanta with energy $\hbar\omega(k)$ above that of the ground state.

4.3.3 Many Particle States

If we define the *occupation number operator* $\hat{n}(k)$ by

$$\hat{n}(k) = \hat{a}^\dagger(k)\hat{a}(k) \quad (4.107)$$

i.e., the quantum number of the k -th oscillator, we see that the most general eigenstate is labelled by the set of oscillator quantum numbers $\{n(k)\}$. Thus, the state $|\{n(k)\}\rangle$ defined by

$$|\{n(k)\}\rangle = \prod_k \frac{[\hat{a}^\dagger(k)]^{n(k)}}{\sqrt{n(k)!}} |0\rangle \quad (4.108)$$

has energy $E[\{n(k)\}]$

$$E[\{n(k)\}] = \int_{-\pi}^{\pi} \frac{dk}{2\pi} n(k) \hbar \omega(k) + E_0 \quad (4.109)$$

It is clear that the excitations behave as *free particles* since their energies are additive. These excitations are known as phonons. They are the quantized fluctuations of the array of atoms.

4.4 Quantization of the Free Scalar Field Theory

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

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{1}{2}m^2 \phi^2 \quad (4.110)$$

This system can be studied using methods which are almost identical to the ones we used in our discussion of the chain of atoms of the previous section.

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

$$\hat{H} = \int d^3x \left[\frac{1}{2} \hat{\Pi}^2(\mathbf{x}) + \frac{1}{2} (\nabla \hat{\phi}(\mathbf{x}))^2 + \frac{1}{2} m^2 \hat{\phi}^2(\mathbf{x}) \right] \quad (4.111)$$

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

$$[\hat{\phi}(\mathbf{x}, x_0), \hat{\Pi}(\mathbf{y}, x_0)] = i\delta(\mathbf{x} - \mathbf{y}) \quad (4.112)$$

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

$$\begin{aligned} i\partial_0 \hat{\phi}(\mathbf{x}, x_0) &= [\hat{\phi}(\mathbf{x}, x_0), \hat{H}] \\ i\partial_0 \hat{\Pi}(\mathbf{x}, x_0) &= [\hat{\Pi}(\mathbf{x}, x_0), \hat{H}] \end{aligned} \quad (4.113)$$

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

$$\partial_0 \hat{\phi}(\mathbf{x}, x_0) = \hat{\Pi}(\mathbf{x}, x_0) \quad (4.114)$$

$$\partial_0 \hat{\Pi}(\mathbf{x}, x_0) = \nabla^2 \hat{\phi}(\mathbf{x}, x_0) - m^2 \hat{\phi}(\mathbf{x}, x_0) \quad (4.115)$$

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

$$(\partial^2 + m^2) \hat{\phi}(x) = 0 \quad (4.116)$$

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

Field Expansion

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

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3} \hat{\phi}(\mathbf{k}, x_0) e^{i\mathbf{k}\cdot\mathbf{x}} \quad (4.117)$$

where $\hat{\phi}(\mathbf{k}, x_0)$ are the Fourier amplitudes of $\hat{\phi}(x)$. We now demand that the $\hat{\phi}(x)$ satisfies the Klein-Gordon equation, and find that $\hat{\phi}(\mathbf{k}, x_0)$ should satisfy

$$\partial_0^2 \hat{\phi}(\mathbf{k}, x_0) + (\mathbf{k}^2 + m^2) \hat{\phi}(\mathbf{k}, x_0) = 0 \quad (4.118)$$

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

$$\hat{\phi}^\dagger(\mathbf{k}, x_0) = \hat{\phi}(-\mathbf{k}, x_0) \quad (4.119)$$

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

$$\hat{\phi}(\mathbf{k}, x_0) = \hat{\phi}_+(\mathbf{k}) e^{i\omega(\mathbf{k})x_0} + \hat{\phi}_-(\mathbf{k}) e^{-i\omega(\mathbf{k})x_0} \quad (4.120)$$

The operators $\hat{\phi}_+(\mathbf{k})$ and $\hat{\phi}_+^\dagger(\mathbf{k})$ are not independent since the reality condition implies that

$$\hat{\phi}_+(\mathbf{k}) = \hat{\phi}_+^\dagger(-\mathbf{k}) \quad \hat{\phi}_+^\dagger(\mathbf{k}) = \hat{\phi}_+(-\mathbf{k}) \quad (4.121)$$

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

$$\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m^2} \quad (4.122)$$

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

$$\hat{a}(\mathbf{k}) = 2\omega(\mathbf{k}) \hat{\phi}_-(\mathbf{k}) \quad \hat{a}^\dagger(\mathbf{k}) = 2\omega(\mathbf{k}) \hat{\phi}_+^\dagger(\mathbf{k}) \quad (4.123)$$

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

$$[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] = (2\pi)^3 2\omega(\mathbf{k}) \delta^3(\mathbf{k} - \mathbf{k}') \quad (4.124)$$

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

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \left[\hat{a}(\mathbf{k}) e^{-i\omega(\mathbf{k})x_0 + i\mathbf{k}\cdot\mathbf{x}} + \hat{a}^\dagger(\mathbf{k}) e^{i\omega(\mathbf{k})x_0 - i\mathbf{k}\cdot\mathbf{x}} \right] \quad (4.125)$$

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

The canonical momentum also can be expanded in a similar way

$$\hat{\Pi}(x) = -i \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \omega(k) \left[\hat{a}(\mathbf{k}) e^{-i\omega(\mathbf{k})x_0 + i\mathbf{k}\cdot\mathbf{x}} - \hat{a}^\dagger(\mathbf{k}) e^{i\omega(\mathbf{k})x_0 - i\mathbf{k}\cdot\mathbf{x}} \right] \quad (4.126)$$

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

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \quad (4.127)$$

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

We will now follow the same approach that we used for the problem of the linear chain and write the Hamiltonian in terms of the operators $\hat{a}(\mathbf{k})$ and $\hat{a}^\dagger(\mathbf{k})$. The result is

$$\hat{H} = \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \frac{\omega(\mathbf{k})}{2} \left(\hat{a}(\mathbf{k})\hat{a}^\dagger(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}) \right) \quad (4.128)$$

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

Ground State

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

$$\hat{a}(\mathbf{k})|0\rangle = 0 \quad (4.129)$$

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

$$\hat{H} =: \hat{H}: + E_0 \quad (4.130)$$

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

$$: \hat{H}: |0\rangle = 0 \quad (4.131)$$

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

$$E_0 = \int d^3k \frac{\omega(\mathbf{k})}{2} \delta(0) \quad (4.132)$$

when $\delta(0)$ is the infrared divergent number

$$\delta(0) = \lim_{p \rightarrow 0} \delta^3(\mathbf{p}) = \lim_{p \rightarrow 0} \int \frac{d^3x}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} = \frac{V}{(2\pi)^3} \quad (4.133)$$

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

$$\varepsilon_0 = \int \frac{d^3k}{(2\pi)^3} \frac{\omega(\mathbf{k})}{2} \equiv \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \sqrt{\mathbf{k}^2 + m^2} \quad (4.134)$$

Eq. (4.134) 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 if the volume is finite. 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 thus it is infinitely large.

It is interesting to compare this issue in the phonon problem with the scalar field theory. In both cases the ground state energy was found to be *extensive*. Thus, the infrared divergence in E_0 was expected in both cases. However, the ultraviolet divergence that we found in the scalar field theory is *absent* in the phonon problem. Indeed, the ground state energy density ε_0 for the linear chain with lattice spacing a is

$$\varepsilon_0 = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{1}{2} \sqrt{\frac{\hbar^2 K}{M} + \frac{4D\hbar^2}{M} \sin^2\left(\frac{ka}{2}\right)} \quad (4.135)$$

Thus integral is *finite* because the momentum integration is limited to the range $|k| \leq \frac{\pi}{a}$. Thus the largest momentum in the chain is $\frac{\pi}{a}$ and it is finite provided that the lattice spacing is not equal to zero. In other words, the integral is *cutoff* by the lattice spacing. However, the scalar field theory that we are considering does not have a cutoff and hence the energy density blows up.

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. 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.

Hilbert Space

We can construct the spectrum of states by inspection of the normal ordered Hamiltonian

$$: \hat{H} := \int \frac{d^3k}{(2\pi)^3} \omega(\mathbf{k}) \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \quad (4.136)$$

This Hamiltonian *commutes* with the *total momentum* $\hat{\mathbf{P}}$

$$\hat{\mathbf{P}} = \int_{x_0 \text{ fixed}} d^3x \hat{\Pi}(\mathbf{x}, x_0) \nabla \hat{\phi}(\mathbf{x}, x_0) \quad (4.137)$$

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

$$\mathbf{P} = \int_{x_0} d^3x T^{0j} \equiv \int_{x_0} d^3x \Pi(\mathbf{x}, x_0) \nabla \phi(\mathbf{x}, x_0) \quad (4.138)$$

In Fourier space $\hat{\mathbf{P}}$ becomes

$$\hat{\mathbf{P}} = \int \frac{d^3k}{(2\pi)^3} \omega(\mathbf{k}) \mathbf{k} \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \quad (4.139)$$

The normal-ordered Hamiltonian $: \hat{H} :$ also commutes with the oscillator occupation number $\hat{n}(\mathbf{k})$, defined by

$$\hat{n}(\mathbf{k}) \equiv \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \quad (4.140)$$

Since $\{\hat{n}(\mathbf{k})\}$ and the Hamiltonian \hat{H} commute with each other, we can use a complete set of eigenstates of $\{\hat{n}(\mathbf{k})\}$ to span the Hilbert space. We will regard the excitations counted by $\hat{n}(\mathbf{k})$ as *particles* that have energy and momentum (and in other theories will also have other quantum numbers).

Their Hilbert space has an indefinite number of particles and it is called *Fock space*. The states $\{|\{n(\mathbf{k})\}\rangle\}$ of the Fock space, defined by

$$|\{n(\mathbf{k})\}\rangle = \prod_{\mathbf{k}} \mathcal{N}(\mathbf{k}) [\hat{a}^\dagger(\mathbf{k})]^{n(\mathbf{k})} |0\rangle, \quad (4.141)$$

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

$$\hat{n}(\mathbf{k})|\{n(\mathbf{k})\}\rangle = (2\pi)^3 2\omega(\mathbf{k}) n(\mathbf{k}) |\{n(\mathbf{k})\}\rangle \quad (4.142)$$

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

The *total number operator* \hat{N}

$$\hat{N} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \hat{n}(\mathbf{k}) \quad (4.143)$$

commutes with the Hamiltonian \hat{H} and it is diagonal in this basis *i.e.*,

$$\hat{N}|\{n(\mathbf{k})\}\rangle = \int d^3k n(\mathbf{k}) |\{n(\mathbf{k})\}\rangle \quad (4.144)$$

The energy of these states is

$$\hat{H}|\{n(\mathbf{k})\}\rangle = \left[\int d^3k n(\mathbf{k}) \omega(\mathbf{k}) + E_0 \right] |\{n(\mathbf{k})\}\rangle \quad (4.145)$$

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

$$\varepsilon(\mathbf{k}) = \int d^3k n(\mathbf{k}) \omega(\mathbf{k}). \quad (4.146)$$

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

$$\hat{\mathbf{P}}|0\rangle = 0. \quad (4.147)$$

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

$$\hat{\mathbf{P}} = \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \mathbf{k} \hat{n}(\mathbf{k}) \quad (4.148)$$

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

$$\hat{\mathbf{P}}|\{n(\mathbf{k})\}\rangle = \left[\int d^3k \mathbf{k} n(\mathbf{k}) \right] |\{n(\mathbf{k})\}\rangle \quad (4.149)$$

The state with lowest energy, the vacuum state $|0\rangle$ has $n(\mathbf{k}) = 0$, for all

\mathbf{k} . Thus the vacuum state has zero momentum and it is translationally invariant.

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

$$|\mathbf{k}\rangle \equiv \hat{a}^\dagger(\mathbf{k})|0\rangle \quad (4.150)$$

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

$$E = \sqrt{\mathbf{k}^2 + m^2}, \quad (4.151)$$

characteristic of a relativistic *particle* of momentum \mathbf{k} and mass m . Thus, the excitations of the ground state of this *field theory* are particle-like. From our discussion we can see that these *particles* are free since their energies and momenta are additive.

Causality

The starting point of the quantization procedure was to impose equal-time commutation relations among the canonical fields $\hat{\phi}(x)$ and momenta $\hat{\Pi}(x)$. 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 $\Delta(x - y)$

$$i\Delta(x - y) = [\hat{\phi}(x), \hat{\phi}(y)] \quad (4.152)$$

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

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \quad (4.153)$$

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

$$\begin{aligned} i\Delta(x - y) = & [\hat{\phi}_+(x), \hat{\phi}_+(y)] + [\hat{\phi}_-(x), \hat{\phi}_-(y)] \\ & + [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] \end{aligned} \quad (4.154)$$

The first two terms always vanish since the $\hat{\phi}_+$ operators commute among

themselves and so do the operators $\hat{\phi}_-$. Thus, we get

$$\begin{aligned} i\Delta(x-y) &= [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] \\ &= \int d\bar{k} \int d\bar{k}' \left\{ [\hat{a}^\dagger(\mathbf{k}), \hat{a}(\mathbf{k}')] \exp(-i\omega(k)x_0 + i\mathbf{k} \cdot \mathbf{x} + i\omega(k')y_0 - i\mathbf{k}' \cdot \mathbf{y}) \right. \\ &\quad \left. + [\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] \exp(i\omega(k)x_0 - i\mathbf{k} \cdot \mathbf{x} - i\omega(k')y_0 + i\mathbf{k}' \cdot \mathbf{y}) \right\} \end{aligned} \quad (4.155)$$

where

$$\int d\bar{k} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \quad (4.156)$$

By using the commutation relations, 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

$$i\Delta(x-y) = \int d\bar{k} \left[e^{i\omega(\mathbf{k})(x_0-y_0) - i\mathbf{k} \cdot (\mathbf{x}-\mathbf{y})} - e^{-i\omega(\mathbf{k})(x_0-y_0) + i\mathbf{k} \cdot (\mathbf{x}-\mathbf{y})} \right] \quad (4.157)$$

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

$$\epsilon(k^0) = \frac{k^0}{|k^0|} \equiv \text{sign}(k^0) \quad (4.158)$$

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

$$i\Delta(x-y) = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 - m^2) \epsilon(k^0) e^{-ik \cdot (x-y)} \quad (4.159)$$

The integrand vanishes unless the *mass shell condition*

$$k^2 - m^2 = 0 \quad (4.160)$$

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

$$\partial_0 \Delta|_{x_0=y_0} = -\delta^3(\mathbf{x}-\mathbf{y}) \quad (4.161)$$

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

$$\Delta(\mathbf{x}-\mathbf{y}, 0) = 0 \quad (4.162)$$

Furthermore, it 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 $(x-y)^2 = (x_0-y_0)^2 - (\mathbf{x}-\mathbf{y})^2 = -(\mathbf{x}-\mathbf{y})^2 < 0$, 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 (for details see Fig.4.3).

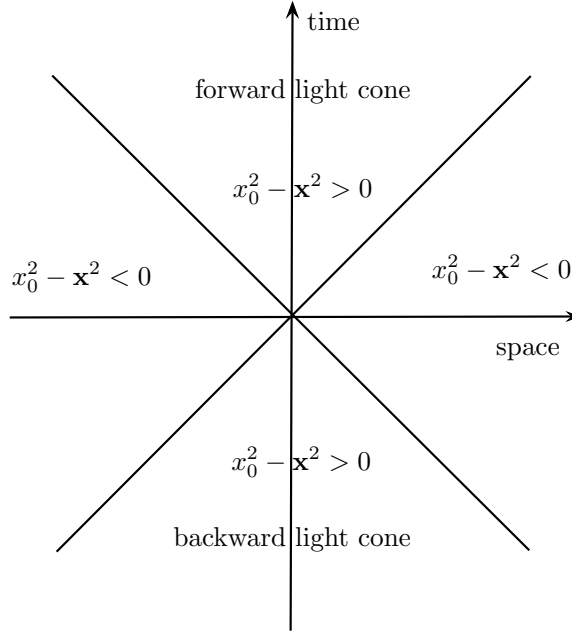


Figure 4.3 The Minkowski space-time.

4.5 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. It is then natural to ask what role do 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

$$\frac{dA}{dt} = \{A, H\}_{PB} = 0 \quad (4.163)$$

in the quantum theory becomes the operator identity

$$i\frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}] = 0 \quad (4.164)$$

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

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

$$\hat{Q} = \int_{x_0 \text{ fixed}} d^3x \hat{j}^0(\mathbf{x}, x_0) \quad (4.165)$$

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

$$[\hat{Q}, \hat{H}] = 0 \quad (4.166)$$

If this is so, the charges \hat{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 $\hat{U}(\alpha)$ associated with the symmetry

$$\hat{U}(\alpha) = \exp(i\alpha\hat{Q}) \quad (4.167)$$

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

$$P^\mu = \int_{x_0} d^3x T^{0\mu} \quad (4.168)$$

is conserved. In the quantum theory P^0 becomes the Hamiltonian operator \hat{H} and $\hat{\mathbf{P}}$ is the total momentum operator. In the case of a free scalar field we saw before that these operators commute with each other, $[\hat{\mathbf{P}}, \hat{H}] = 0$. Thus, the eigenstates of the system have well defined total energy and total momentum. Since \mathbf{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

$$\{\phi(\mathbf{x}, x_0), P^j\}_{PB} = \partial_x^j \phi \quad (4.169)$$

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

$$[\hat{\phi}(\mathbf{x}, x_0), \hat{P}^j] = i\partial_x^j \hat{\phi}(\mathbf{x}, x_0) \quad (4.170)$$

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

$$\hat{\phi}(\mathbf{x} + \mathbf{a}, x_0) = e^{i\mathbf{a}\cdot\hat{\mathbf{P}}} \hat{\phi}(\mathbf{x}, x_0) e^{-i\mathbf{a}\cdot\hat{\mathbf{P}}} \quad (4.171)$$

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

$$e^{i\mathbf{a}\cdot\hat{\mathbf{P}}}|0\rangle = |0\rangle \quad (4.172)$$

which states that the state $|0\rangle$ is invariant 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 be decomposed into its real and imaginary parts

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \quad (4.173)$$

The classical Lagrangian for a free complex scalar field ϕ is

$$\mathcal{L} = \partial_\mu\phi^*\partial^\mu\phi - m^2\phi^*\phi \quad (4.174)$$

now splits into a sum of two independent terms

$$\mathcal{L}(\phi) = \mathcal{L}(\phi_1) + \mathcal{L}(\phi_2) \quad (4.175)$$

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

$$\Pi(x) = \frac{\delta\mathcal{L}}{\delta\dot{\phi}} = \frac{1}{\sqrt{2}}(\dot{\phi}_1 - i\dot{\phi}_2) \quad \Pi^*(x) = \frac{1}{\sqrt{2}}(\dot{\phi}_1 + i\dot{\phi}_2) \quad (4.176)$$

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

$$[\hat{\phi}(\mathbf{x}, x_0), \hat{\Pi}(\mathbf{y}, x_0)] = i\delta^3(\mathbf{x} - \mathbf{y}) \quad (4.177)$$

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

$$\begin{aligned} \hat{a}(\mathbf{k}) &= \frac{1}{\sqrt{2}}(\hat{a}_1(\mathbf{k}) + i\hat{a}_2(\mathbf{k})), & \hat{a}^\dagger(\mathbf{k}) &= \frac{1}{\sqrt{2}}(\hat{a}_1^\dagger(\mathbf{k}) - i\hat{a}_2^\dagger(\mathbf{k})) \\ \hat{b}(\mathbf{k}) &= \frac{1}{\sqrt{2}}(\hat{a}_1(\mathbf{k}) - i\hat{a}_2(\mathbf{k})), & \hat{b}^\dagger(\mathbf{k}) &= \frac{1}{\sqrt{2}}(\hat{a}_1^\dagger(\mathbf{k}) + i\hat{a}_2^\dagger(\mathbf{k})) \end{aligned} \quad (4.178)$$

which satisfy the algebra

$$[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] = [\hat{b}(\mathbf{k}), \hat{b}^\dagger(\mathbf{k}')] = (2\pi)^3 2\omega(\mathbf{k}) \delta^3(\mathbf{k} - \mathbf{k}') \quad (4.179)$$

while all other commutators vanish.

The Fourier expansion for the fields now is

$$\begin{aligned} \hat{\phi}(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \left(\hat{a}(\mathbf{k}) e^{-ik \cdot x} + \hat{b}^\dagger(\mathbf{k}) e^{ik \cdot x} \right) \\ \hat{\phi}^\dagger(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \left(\hat{b}(k) e^{-ik \cdot x} + \hat{a}^\dagger(k) e^{ik \cdot x} \right) \end{aligned} \quad (4.180)$$

where $\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m^2}$ and $k_0 = \omega(\mathbf{k})$.

The normal ordered Hamiltonian is

$$: \hat{H} := \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \omega(\mathbf{k}) \left(\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) + \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k}) \right) \quad (4.181)$$

and the normal-ordered total linear momentum $\hat{\mathbf{P}}$ is

$$\hat{\mathbf{P}} = \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \mathbf{k} \left(\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) + \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k}) \right) \quad (4.182)$$

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.

The one-particle states have now a two-fold degeneracy since the states $\hat{a}^\dagger(\mathbf{k})|0\rangle$ and $\hat{b}^\dagger(\mathbf{k})|0\rangle$ have one particle of type a and one of type b respectively but these states have exactly the same energy, $\omega(\mathbf{k})$, and the same momentum \mathbf{k} . Thus for each value of the energy and of the 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

$$j_\mu = i\phi^* \overset{\leftrightarrow}{\partial}_\mu \phi \quad (4.183)$$

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

$$\begin{aligned} \hat{Q} &= : \int d^3x i \left(\hat{\phi}^\dagger \partial_0 \hat{\phi} - (\partial_0 \hat{\phi}^\dagger) \hat{\phi} \right) : \\ &= \int \frac{d^3k}{(2\pi)^3 2\omega(\mathbf{k})} \left(\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) - \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k}) \right) \\ &= \hat{N}_a - \hat{N}_b \end{aligned} \quad (4.184)$$

where \hat{N}_a and \hat{N}_b are the number operators for quanta of type a and b respectively. Since $[\hat{Q}, \hat{H}] = 0$, 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 $[\hat{Q}, \hat{H}] = 0$. 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.

Vacuum State

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

$$\hat{Q}|0\rangle = 0 \quad (4.185)$$

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

$$|0\rangle' = e^{i\hat{Q}\alpha}|0\rangle = |0\rangle \quad (4.186)$$

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, it is trivial.

One-particle States

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

$$|+, \mathbf{k}\rangle = \hat{a}^\dagger(\mathbf{k})|0\rangle \quad |-, \mathbf{k}\rangle = \hat{b}^\dagger(\mathbf{k})|0\rangle \quad (4.187)$$

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

$$\begin{aligned} \hat{Q}|+, \mathbf{k}\rangle &= (\hat{N}_a - \hat{N}_b)\hat{a}^\dagger(\mathbf{k})|0\rangle = \hat{N}_a \hat{a}^\dagger(\mathbf{k})|0\rangle = +|+, \mathbf{k}\rangle \\ \hat{Q}|-, \mathbf{k}\rangle &= (\hat{N}_a - \hat{N}_b)\hat{b}^\dagger(\mathbf{k})|0\rangle = -|-, \mathbf{k}\rangle \end{aligned} \quad (4.188)$$

Hence

$$\hat{Q}|\sigma, \mathbf{k}\rangle = \sigma|\sigma, \mathbf{k}\rangle \quad (4.189)$$

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

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

$$\begin{aligned} |+, \mathbf{k}\rangle' &= \hat{U}(\alpha) |+, \mathbf{k}\rangle = \exp(i\alpha\hat{Q}) |+, \mathbf{k}\rangle = e^{i\alpha} |+, \mathbf{k}\rangle \\ |-, \mathbf{k}\rangle' &= \hat{U}(\alpha) |-, \mathbf{k}\rangle = \exp(i\alpha\hat{Q}) |-, \mathbf{k}\rangle = e^{-i\alpha} |-, \mathbf{k}\rangle \end{aligned} \quad (4.190)$$

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

$$\hat{\phi}'(x) = \exp(-i\alpha\hat{Q}) \hat{\phi}(x) \exp(i\alpha\hat{Q}) = e^{i\alpha} \hat{\phi}(x) \quad (4.191)$$

since

$$[\hat{Q}, \hat{\phi}(x)] = -\hat{\phi}(x), \quad [\hat{Q}, \hat{\phi}^\dagger(x)] = \hat{\phi}^\dagger(x) \quad (4.192)$$

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

By inspecting 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 $|\pm, \mathbf{k}\rangle$ are commonly referred to as *particles* and *antiparticles*: particles have rest mass m , momentum \mathbf{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).

Let us finally note that this theory contains an additional operator, the charge conjugation operator \hat{C} , which maps particles into antiparticles and vice versa. This operator commutes with the Hamiltonian, $[\hat{C}, \hat{H}] = 0$. 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 \hat{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 non-linear or interacting theories. We will return to this important question later on.