4 Canonical Quantization

We will begin now the discussion of our main subject of interest: the role of quantum mechanical fluctuations in systems with infintely 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 key ingredients 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:

$$p = \frac{\partial L}{\partial \dot{q}} \tag{1}$$

In this approach, the dynamics of the system is governed by the classical Hamiltonian

$$H(q,p) = p\dot{q} - L(q,\dot{q}) \tag{2}$$

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

$$\dot{p} = -\frac{\partial H}{\partial q} \qquad \dot{q} = \frac{\partial H}{\partial p} \tag{3}$$

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

$$\{q,p\}_{PB} = 1 \qquad \{q,q\}_{PB} = \{p,p\}_{PB} = 0 \tag{4}$$

where

$$\{A,B\}_{PB} \equiv \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} \tag{5}$$

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 *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.,* $|a\Psi + b\Phi\rangle \in \mathcal{H}$. Thus, the *Superposition Principle* is an axiom of Quantum Mechanics.

In Quantum Mechanics, the dynamical variables, *i.e.,* $\hat{q}, \hat{p}, H$, *etc.* , are represented by *operators* which act *linearly* on the Hilbert space of states. (In this sense, Quantum Mechanics is linear, even though the observables obey non-linear equations of motion.) Let us denote by $\hat{A}$ an arbitrary operator acting on $\mathcal{H}$. The result of acting on the state $|\Psi\rangle \in \mathcal{H}$ with the operator $\hat{A}$, *i.e.,* a *measurement*, is another state $|\Phi\rangle \in \mathcal{H}$,

$$\hat{A}|\Psi\rangle = |\Phi\rangle \tag{6}$$

The Hilbert space $\mathcal{H}$ is endowed with an *inner product*. An inner product is an operation which 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,* which spans the entire Hilbert space. Thus, an arbitrary state $|\Psi\rangle$ has the expansion

$$|\Psi\rangle = \sum_{\lambda} \Psi_\lambda \; |\lambda\rangle \tag{7}$$

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

$$\langle\lambda|\mu\rangle = \delta_{\lambda\mu} \tag{8}$$

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

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1 \tag{9}$$

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

$$\hat{A}|\Psi\rangle = \alpha|\Phi\rangle \tag{10}$$

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

$$\alpha = \langle\Phi|\hat{A}|\Psi\rangle \tag{11}$$

Operators which 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 the classical limit, $\hbar \to 0$, the operators should 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), which satisfies the Poisson Bracket $\{q, p\}_{PB} = 1$, we associate a *pair of operators* $\hat{q}$ and $\hat{p}$, both acting on the Hilbert space of states $\mathcal{H}$, which are *required* to obey the *canonical commutation relations*

$$[\hat{q}, \hat{p}] = i\hbar \qquad [\hat{q}, \hat{q}] = [\hat{p}, \hat{p}] = 0 \tag{12}$$

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

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{13}$$

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

To the classical Hamiltonian $H(q,p)$, which is a *function* of the variables q and p, we assign an *operator* $\hat{H}(\hat{q},\hat{p})$ which is obtained by replacing the dynamical variables with the corresponding operators. Other classical dynamical quantities are similarly associated with quantum operators. All operators associated with classical physical quantities 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 $\hat{A}$

$$\langle\Psi|\hat{A}^\dagger|\Phi\rangle \equiv \langle\Phi|\hat{A}\Psi\rangle^* \tag{14}$$

then $\hat{A}$ is Hermitian if $\hat{A} = \hat{A}^\dagger$.

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

$$i\hbar\frac{\partial}{\partial t}\,|\Phi(t)\rangle = \hat{H}(\hat{q},\hat{p})\,|\Psi(t)\rangle \tag{15}$$

The state $|\Psi(t)\rangle$ is uniquely determined by the initial state $|\Psi(0)\rangle$.

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

$$\hat{q}|q\rangle = q\,|q\rangle \tag{16}$$

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

$$|\Psi\rangle = \sum_q \Psi(q)\,|q\rangle = \int_{-\infty}^{+\infty} dq\;\Psi(q)\,|q\rangle \tag{17}$$

The coefficients $\Psi(q)$ of this expansion

$$\Psi(q) = \langle q|\Psi\rangle \tag{18}$$

are (the values of) the *wave function* associated with the state $|\Psi\rangle$ in the *coordinate representation*. Here we have used that the states $|q\rangle$ are *orthonormal* and *complete*, *i. e.*

$$\langle q|q'\rangle = \delta(q-q') \qquad \hat{I} = \int dq\;|q\rangle\langle q| \tag{19}$$

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

$$\hat{q}\ \exp(\frac{-i}{\hbar}a\hat{p})\ |q\rangle \equiv \hat{q}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-ia}{\hbar}\right)^{n}\ \hat{p}^{n}\ |q\rangle \tag{20}$$

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

$$[\hat{q},\hat{p}^{n}] = i\hbar n\hat{p}^{n-1} \tag{21}$$

Hence, we can write

$$\hat{q}\ \exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle = (q+a)\exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle \tag{22}$$

Thus,

$$\exp\left(-\frac{i}{\hbar}a\hat{p}\right)|q\rangle = |q+a\rangle \tag{23}$$

We can now use this property to compute the matrix element

$$\langle q|\exp\left(\frac{i}{\hbar}a\hat{p}\right)|\Psi\rangle \equiv \Psi(q+a) \tag{24}$$

For a infinitesimally small, it can be approximated by

$$\Psi(q+a) \approx \Psi(q) + \frac{i}{\hbar}a\langle q|\hat{p}|\Psi\rangle + \ldots \tag{25}$$

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

$$\langle q|\hat{p}|\Psi\rangle = \frac{\hbar}{i}\lim_{a\to 0}\frac{\Psi(q+a)-\Psi(q)}{a} \tag{26}$$

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

$$\langle q|\hat{p}|\Psi\rangle \equiv \frac{\hbar}{i}\frac{\partial}{\partial q}\Psi(q) = \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q|\Psi\rangle \tag{27}$$

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

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial q} \tag{28}$$

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, *i.e.,*

$$\Pi(x) = \frac{\partial \mathcal{L}}{\delta \partial_0 \phi(x)} \tag{29}$$

On a given time surface x_0, the classical Hamiltonian is

$$H = \int d^3x \ \left[\Pi(\vec{x}, x_0) \partial_0 \phi(\vec{x}, x_0) - \mathcal{L}(\phi, \partial_\mu \phi)\right] \tag{30}$$

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 $\phi(\vec{x})$ and the canonical momentum $\Pi(\vec{x})$ are operators which act on a Hilbert space. These operators obey *canonical commutation relations*

$$[\phi(\vec{x}), \Pi(\vec{y})] = i\hbar \delta(\vec{x} - \vec{y}) \tag{31}$$

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

$$\Psi = \Psi(\{\phi(\vec{x})\}) \equiv \langle \{\phi(\vec{x})\} | \Psi \rangle \tag{32}$$

In this representation, the field is a diagonal operator

$$\langle \{\phi\} | \hat{\phi}(\vec{x}) | \Psi \rangle \equiv \phi(\vec{x}) \ \langle \{\phi(\vec{x})\} | \Psi \rangle = \phi(\vec{x}) \ \Psi(\{\phi\}) \tag{33}$$

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

$$\langle \{\phi\} | \hat{\Pi}(\vec{x}) | \Psi \rangle \equiv \frac{\hbar}{i} \frac{\delta}{\delta \phi(\vec{x})} \Psi(\{\phi\}) \tag{34}$$

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

$$i\hbar \frac{\partial}{\partial t} \Psi(\{\phi\}, t) = \hat{H} \Psi(\{\phi\}, t). \tag{35}$$

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

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \phi)^2 - V(\phi) \tag{36}$$

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

$$\hat{H} = \int d^3x \ \left\{ \frac{1}{2} \hat{\Pi}^2(\vec{x}) + \frac{1}{2} (\vec{\bigtriangledown} \hat{\phi}(\vec{x}))^2 + V(\vec{\phi}(\vec{x})) \right\} \tag{37}$$

The stationary states of the system are the eigenstates of $\hat{H}$. 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 information on 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 not. The operators of the Heisenberg Picture obey quantum mechanical equations of motion.

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

$$\hat{A}_H(x_0) = e^{\frac{i}{\hbar}\hat{H}x_0}\ \hat{A}\ e^{-\frac{i}{\hbar}\hat{H}x_0} \tag{38}$$

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

$$i\hbar\partial_0\hat{A}_H(x_0) = [\hat{A}_H(x_0), \hat{H}] \tag{39}$$

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

$$\partial_0 A(x_0) = \{A(x_0), H\}_{PB} \tag{40}$$

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 $\hat{\phi}(\vec{x}, x_0)$ and $\hat{\Pi}(\vec{x}, x_0)$ are time dependent operators which obey the equations of motion

$$i\hbar\partial_0\hat{\phi} = \left[\hat{\phi}, \hat{H}\right] \tag{41}$$

and

$$i\hbar\partial_0\hat{\Pi} = [\hat{\Pi}, \hat{H}] \tag{42}$$

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

$$\left[\hat{\phi}(\vec{x}, x_0), \hat{\Pi}(\vec{y}, x_0)\right] = i\hbar\delta(\vec{x} - \vec{y}) \tag{43}$$

4.3 Quantized elastic waves in a solid: Phonons

Let us consider the problem of the quantum dynamics of an array of atoms. 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 $x_n^0 = na_0, (n = 1, \ldots, n)$ where a_0 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 $L = Na_0$. To simplify matters, I will assume that the chain is actually a ring and, thus, the $N + 1 - st$ atom is the

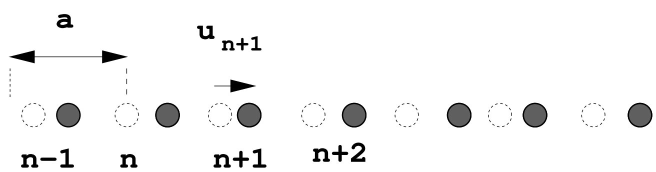

Figure 1: A model of an elastic one-dimensional solid.

same as the 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 $\{u_n\}$, 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 the potential energy, *i.e.,*

$$L(\{u_n\}, \{\dot{u}_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \frac{M}{2} \left(\frac{du_n}{dt} \right)^2 - V(\{u_n\}) \tag{44}$$

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

$$V(\{u_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} [\frac{D}{2}(u_{n+1} - u_n)^2 + \frac{K}{2} u_n^2 + \ldots] \tag{45}$$

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, $u_n \to u_n + a$. The term proportional to u_n^2 breaks this symmetry, although it does not spoil the symmetry $n \to n + m$.

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

$$p_n(t) = \frac{\partial L}{\partial \dot{u}_n(T)} = M \dot{u}_n(t) \tag{46}$$

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

$$H(\{\hat{u}_n\},\{\hat{p}_n\}) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left[\frac{\hat{p}_n^2}{2M} + \frac{D}{2}(\hat{u}_{n+1}-\hat{u}_n)^2 + \frac{K}{2}\hat{u}_n^2 + \cdots \right] \tag{47}$$

where the coordinates and momenta obey the commutation relations

$$[\hat{u}_n, \hat{p}_m] = i\hbar\delta_{n,m} \tag{48}$$

and

$$[\hat{u}_n, \hat{u}_m] = [\hat{p}_n, \hat{p}_m] = 0. \tag{49}$$

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

$$|\Psi\rangle = |\Psi\rangle_1 \otimes \cdots \otimes |\Psi\rangle_n \otimes \cdots \otimes |\Psi\rangle_N \equiv |\Psi_1, \ldots, \Psi_N\rangle \tag{50}$$

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

$$\hat{u}_n|u_n\rangle = u_n|u_n\rangle \tag{51}$$

we can write a set of basis states

$$|u_1, \ldots, u_N\rangle \tag{52}$$

of the form

$$|u_1, \ldots, u_N\rangle = |u_1\rangle \otimes \cdots \otimes |u_N\rangle \tag{53}$$

In this basis, the wave functions are

$$\Psi(u_1, \ldots, u_N) = \langle u_1, \ldots, u_N|\Psi\rangle = \prod_{n=1}^{N} \langle u_n|\Psi_n\rangle = \prod_{n=1}^{N} \Psi_n(u_n) \tag{54}$$

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

$$\hat{u}_n = \frac{1}{N}\sum_k \tilde{u}_k \, e^{ikn} \tag{55}$$

where k is a label (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.,* the chain in a ring) means that

$$\hat{u}_n = \hat{u}_{n+N} \tag{56}$$

This relation can hold only if the labels k satisfy

$$e^{ikN} = 1 \tag{57}$$

This condition restricts the values of k to the *discrete* set

$$k_m = 2\pi \frac{m}{N} \qquad m = -\frac{N}{2} + 1, \ldots, \frac{N}{2} \tag{58}$$

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

$$\hat{u}_n = \frac{1}{N} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \tilde{u}_{k_m} \; e^{ik_m n} \tag{59}$$

The spacing Δk between two consecutive values of k, k_m and k_{m+1}, is

$$\Delta k = k_{m+1} - k_m = \frac{2\pi}{N} \tag{60}$$

which vanishes as $N \to \infty$. 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 $N \to \infty$ the momenta fill up densly the interval $(-\pi, \pi]$.

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

$$\hat{u}_n = \lim_{N \to \infty} \frac{1}{N} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \tilde{u}_{k_m} \; e^{ik_m n} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \; \tilde{u}(k) \; e^{ikn} \tag{61}$$

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

$$\tilde{u}^{\dagger}(k) = \tilde{u}(-k) \tag{62}$$

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

$$\tilde{u}(k) = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \hat{u}_n \; e^{-ikn} \tag{63}$$

where I have used the periodic Dirac delta function, defined by

$$\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{i(k-q)n} = \sum_{m=-\infty}^{+\infty} 2\pi\delta(k - q + 2\pi m) \equiv 2\pi\delta_P(k - q) \tag{64}$$

which is defined in the thermodynamic limit.

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

$$\hat{p}_n = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \; \tilde{p}(k) \; e^{ikn} \qquad \tilde{p}(k) = \sum_{n=-\frac{N}{2+1}}^{\frac{N}{2}} e^{-ikn} \; \hat{p}_n \tag{65}$$

They satisfy

$$\tilde{p}^{\dagger}(k) = \tilde{p}(-k) \tag{66}$$

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

$$\begin{aligned} [\tilde{u}(k), \tilde{p}(k')] &= \sum_{n,n'=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-i(kn+k'n')} \, [\tilde{u}_n, \tilde{p}_{n'}] \\ &= i\hbar \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-i(k+k')n} \end{aligned} \tag{67}$$

Hence, we find

$$[\tilde{u}(k), \tilde{p}(k')] = i\hbar \, 2\pi \, \delta_P(k+k') \tag{68}$$

and

$$[\tilde{u}(k), \tilde{p}(k')] = [\tilde{p}(k), \tilde{p}(k')] = 0 \tag{69}$$

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

$$H = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \, [\frac{1}{2M} \tilde{p}^{\dagger}(k)\tilde{p}(k) + \frac{M}{2}\omega^2(k)\tilde{u}^{\dagger}(k)\tilde{u}(k)] \tag{70}$$

where $\omega^2(k)$ is

$$\omega^2(k) = \frac{K}{M} + \frac{4D}{M} \sin^2(\frac{k}{2}) \tag{71}$$

Thus, the system decouples into its normal modes. The frequency $\omega(k)$ is shown in the figure 2. It is instructive to study the long-wave length limit, $k \to 0$. For $K = 0$ (*i.e.,* no external potential), $\omega(k)$ goes to zero linearly as $k \to 0$,

$$\omega(k) \approx \sqrt{\frac{D}{M}} \, |k| \qquad (K=0) \tag{72}$$

However, for non-zero K, we get (again in the limit $k \to 0$)

$$\omega(k) \approx \sqrt{\frac{K}{M} + \frac{D}{M} k^2} \tag{73}$$

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

$$\omega(\tilde{k}) = v_s \, \sqrt{\bar{m}^2 v_s^2 + \tilde{k}^2} \tag{74}$$

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

$$v_s = \sqrt{\frac{D}{M}} \, a_0 \equiv \sqrt{\frac{D a_0}{\bar{\rho}}} \tag{75}$$

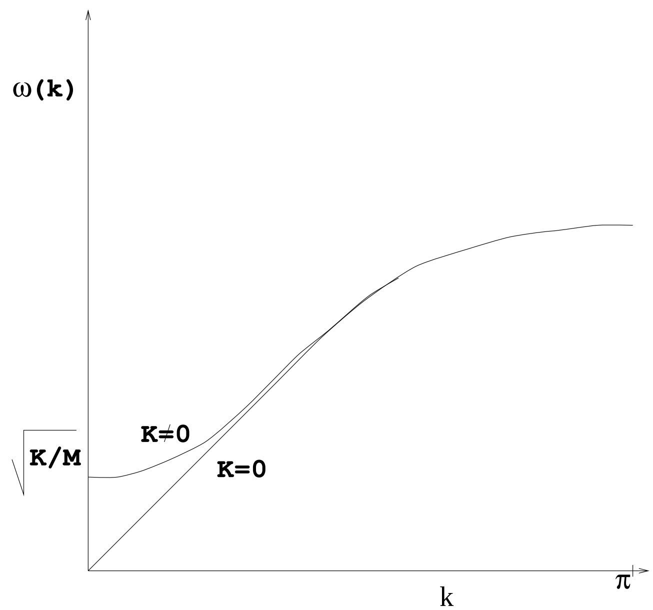

Figure 2: The dispersion relation.

where $\bar{\rho}$ is the density. The "mass" $\bar{m}$ is

$$\bar{m} = \frac{\omega_0}{v_s^2} \tag{76}$$

where $\omega_0 = \sqrt{\frac{K}{M}}$. Thus, the waves which propagate on this chain behave like "relativistic" particles with mass $\bar{m}$ and "speed of light" v_s. Indeed, the long wavelength limit ($k \to 0$) the discrete Lagrangian of eq (4.3.1) can be written in the form of an integral

$$L = a_0 \sum_n \frac{1}{2} \left(\frac{M}{a_0} \right) \left(\frac{\partial u_n}{\partial t} \right)^2 - \frac{a_0}{2} \sum_n D a_0 \left(\frac{u_{n+1} - u_n}{a_0} \right)^2 - \frac{a_0}{2} \sum_n \frac{K}{a_0} u_n^2 \tag{77}$$

Thus, as $a_0 \to 0$ and $N \to \infty$, the sums converge to an integral

$$L = \bar{\rho} \int_{-\frac{\ell}{2}}^{\ell/2} dx \; \{ \frac{1}{2} \left(\frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} v_s^2 \left(\frac{\partial u}{\partial x} \right)^2 - \frac{1}{2} \bar{m}^2 v_s^4 u^2(x) \} \tag{78}$$

for a system of total length ℓ. Apart 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 (KG) field $u(x)$ in one-space dimension. The last term of this Lagrangian is precisely the mass term for the Lagrangian of the KG field. This explains the choice of the symbol $\bar{m}$. Indeed, upon the change of variables

$$x_0 = v_s t \qquad x_1 = x \tag{79}$$

and by defining the rescaled field

$$\varphi = \sqrt{\bar{\rho} v_s}\, u \tag{80}$$

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

$$\mathcal{L} = \frac{1}{2}\left(\partial_0 \varphi\right)^2 - \frac{1}{2}\left(\partial_1 \varphi\right)^2 - \frac{1}{2}\bar{m}^2 v_s^2 \varphi^2 \tag{81}$$

which is the Lagrangian density for a free scalar field in one spacial dimension.

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

$$\begin{aligned} \hat{a}^\dagger(k) &= \frac{1}{\sqrt{2M\hbar\omega(k)}} \left(M\omega(k)\tilde{u}^\dagger(k) - i\tilde{p}^\dagger(k)\right) \\ \hat{a}(k) &= \frac{1}{\sqrt{2M\hbar\omega(k)}} \left(M\omega(k)\tilde{u}(k) + i\tilde{p}(k)\right) \end{aligned} \tag{82}$$

These operators satisfy the commutation relations

$$\begin{aligned} \left[\hat{a}(k), \hat{a}(k')\right] &= \left[\hat{a}^\dagger(k), \hat{a}^\dagger(k')\right] = 0 \\ \left[\hat{a}(k), \hat{a}^\dagger(k')\right] &= 2\pi\delta_P(k+k') \end{aligned} \tag{83}$$

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

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

$$\begin{aligned} \tilde{u}(k) &= \sqrt{\frac{\hbar}{2M\omega(k)}}\, \left(\hat{a}(k) + \hat{a}^\dagger(-k)\right) \\ \tilde{p}(k) &= \sqrt{2M\hbar\omega(k)}\, \frac{1}{2i} \left(\hat{a}(k) - \hat{a}^\dagger(-k)\right) \end{aligned} \tag{84}$$

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

$$\begin{aligned} \hat{u}_n &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sqrt{\frac{\hbar}{2M\omega(k)}}\, \left(\hat{a}(k)\, e^{ikn} + \hat{a}^\dagger(k)\, e^{-ikn}\right) \\ \hat{p}_n &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sqrt{2M\hbar\omega(k)}\, \frac{1}{2i} \left(\hat{a}(k)\, e^{ikn} - \hat{a}^\dagger(k)\, e^{-ikn}\right) \end{aligned} \tag{85}$$

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

$$H = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} \left(\hat{a}^{\dagger}(k)\hat{a}(k) + \hat{a}(k)\hat{a}^{\dagger}(k) \right) \tag{86}$$

It is customary to write H in such a way that the creation operators always appear *to the left* of anihilation 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 eq (4.3.39), we get

$$\hat{a}(k)\hat{a}^{\dagger}(k) = [\hat{a}(k), \hat{a}^{\dagger}(k)] + \hat{a}^{\dagger}(k)\hat{a}(k) \tag{87}$$

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

$$\begin{aligned} [\hat{a}(k), \hat{a}^{\dagger}(k)] &= \lim_{k' \to k} 2\pi\delta_P(k - k^{'}) = \lim_{k' \to k} 2\pi \sum_{m=\infty}^{+\infty} \delta(k - k^{'} + 2\pi m) \\ &= \lim_{k' \to k} \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} e^{i(k-k^{'})n} = N \end{aligned} \tag{88}$$

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

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

$$\hat{H} =: \hat{H} : +E_0 \tag{89}$$

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

$$:\hat{H}:= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \; \hbar\omega(k) \; \hat{a}^{\dagger}(k)\hat{a}(k) \tag{90}$$

and the real number E_0 is given by

$$E_0 = N \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} \tag{91}$$

We will see below that E_0 is the ground state energy of this system. The linear divergence of E_0 (as $N \to \infty$) is natural since the ground state energy has to be an *extensive* quantity, *i.e.,* it scales like the length (volume) of the chain (system).

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

1. *Ground state*:
   Let $|0\rangle$ be the state which is anihilated by all the operators $\hat{a}(k)$,

$$\hat{a}(k)|0\rangle = 0 \tag{92}$$

This state is an eigenstate with eigenvalue E_0 since

$$\hat{H}|0\rangle =: \hat{H} : |0\rangle + E_0|0\rangle = E_0|0\rangle \tag{93}$$

where we have used the fact that $|0\rangle$ is anihilated by the normal-ordered Hamilitonian $:\hat{H}:$. 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 $\Psi_0\left(\{\hat{u}(k)\}\right) = \langle\{\hat{u}(k)\}|0\rangle$ be the wave function of the ground state. The condition that $|0\rangle$ be anihilated by all the operators $\hat{a}(k)$ means that the matrix element $\langle\{\tilde{u}(k)\}|\hat{a}(k)|0\rangle$ has to vanish. The definition of $\hat{a}(k)$ yields the condition

$$0 = M\omega(k)\ \langle\{\tilde{u}(k)\}|\tilde{u}(k)|0\rangle + i\langle\{\tilde{u}(k)\}|\tilde{p}(k)|0\rangle \tag{94}$$

The commutation relation

$$[\tilde{u}(k), \tilde{p}(k^{'})] = i\hbar\, 2\pi\ \delta_P(k + k^{'}) \tag{95}$$

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

$$\langle\{\tilde{u}(k)|\tilde{p}(k)|0\rangle = \frac{\hbar}{i}\, 2\pi\ \frac{\delta}{\delta\tilde{u}(k)}\ \Psi_0\left(\{\hat{u}(k)\}\right) \tag{96}$$

Thus, the wave functional Ψ_0 must obey the differential equation

$$M\omega(k)\ \hat{u}^*(k)\ \Psi_0\left(\{\hat{u}(k)\}\right) + 2\pi\hbar\ \frac{\delta}{\delta\tilde{u}(k)}\ \Psi_0\left(\{\hat{u}(k)\}\right) = 0 \tag{97}$$

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

$$\Psi_0\left(\{\hat{u}(k)\}\right) = \prod_k \Psi_{0,k}\left(\tilde{u}(k)\right) \tag{98}$$

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

$$M\omega(k)\tilde{u}^*(k)\Psi_{0,k}\left(u(k)\right) + 2\pi\hbar\frac{\partial}{\partial u(k)}\Psi_{0,k}\left(u(k)\right) = 0 \tag{99}$$

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

$$\Psi_{0,k}\left(u(k)\right) = \mathcal{N}(k)\ \exp\left(-\left(\frac{M\omega(k)}{2\pi\hbar}\right)\frac{|\tilde{u}|^2(k)}{2}\right) \tag{100}$$

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

$$\Psi_0(\{\tilde{u}(k)\}) = \mathcal{N}\ \exp[-\int_{-\pi}^{\pi}\frac{dk}{2\pi}\left(\frac{M\omega(k)}{2\pi\hbar}\right)\frac{|\tilde{u}|^2(k)}{2}] \tag{101}$$

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

2. *One-Particle States*:
   Let the ket $|1_k\rangle$ denote the one-particle state
   $$|1_k\rangle \equiv \hat{a}^\dagger(k)|0\rangle \tag{102}$$
   This state is an eigenstate of $\hat{H}$ with eigenvalue $E_1(k)$
   $$\hat{H}|1_k\rangle =: \hat{H}: |1_k\rangle + E_0|1_k\rangle \tag{103}$$
   The normal-ordered term now does give a contribution since
   $$\begin{aligned} :\hat{H}: |1_k\rangle &= \left(\int_{-\pi}^{\pi} \frac{dk'}{2\pi}\; \hbar\omega(k')\; \hat{a}^\dagger(k')\hat{a}(k') \right) \hat{a}^\dagger(k)|0\rangle \\ &= \int_{-\pi}^{\pi} \frac{dk'}{2\pi} \hbar\omega(k^{'}) \{ \hat{a}^\dagger(k')[\hat{a}(k'), \hat{a}^\dagger(k)]|0\rangle + \hat{a}^\dagger(k')\hat{a}^\dagger(k)a(k')|0\rangle \} \end{aligned} \tag{104}$$
   The result is
   $$:\hat{H}: |1_k\rangle = \int_{-\pi}^{\pi} \frac{dk'}{2\pi}\; \hbar\omega(k')\; \hat{a}^\dagger(k')\; 2\pi\delta_P(k'-k)\; |0\rangle \tag{105}$$
   since the last term vanishes. Hence
   $$:\hat{H}: |1_k\rangle = \hbar\omega(k)\; \hat{a}^\dagger(k)\; |0\rangle \equiv \hbar\omega(k)\; |1_k\rangle \tag{106}$$
   Therefore, we find
   $$\hat{H}|1_k\rangle = (\hbar\omega(k) + E_0)\; |1_k\rangle \tag{107}$$
   Let $\varepsilon(k)$ be the excitation energy
   $$\varepsilon(k) \equiv E_1(k) - E_0(k) = \hbar\omega(k) \tag{108}$$
   Thus the one-particle states represent quanta with energy $\hbar\omega(k)$ above that of the ground state.

3. *Many Particle States*:
   If we define the *occupation number operator* $\hat{n}(k)$ by
   $$\hat{n}(k) = \hat{a}^\dagger(k)a(k) \tag{109}$$
   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
   $$|\{n(k)\}\rangle = \prod_k \frac{\left[\hat{a}^\dagger(k)\right]^{n(k)}}{\sqrt{n(k)!}}\; |0\rangle \tag{110}$$
   has energy $E[\{n(k)\}]$
   $$E[\{n(k)\}] = \int_{-\pi}^{\pi} \frac{dk}{2\pi}\; n(k)\hbar\omega(k) + E_0 \tag{111}$$
   It is clear that the excitations behave like *free particles* since the 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 scalar field $\phi(x)$. In particular, we will consider a *free real* scalar field ϕ whose Lagrangian density is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{1}{2}m^2\phi^2 \tag{112}$$

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

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

$$\hat{H} = \int d^3x \, \left[\frac{1}{2}\hat{\Pi}^2(\vec{x}) + \frac{1}{2}\left(\vec{\bigtriangledown}\hat{\phi}(\vec{x})\right)^2 + \frac{1}{2}m^2\hat{\phi}^2(\vec{x})\right] \tag{113}$$

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

$$[\hat{\phi}(\vec{x}, x_0), \hat{\Pi}(\vec{y}, x_0)] = i\delta(\vec{x} - \vec{y}) \tag{114}$$

1. *Equations of Motion*:
   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

   $$\begin{aligned} i\partial_0\hat{\phi}(\vec{x}, x_0) &= [\hat{\phi}(\vec{x}, x_0), \hat{H}] \\ i\partial_0\hat{\Pi}(\vec{x}, x_0) &= [\hat{\Pi}(\vec{x}, x_0), \hat{H}] \end{aligned} \tag{115}$$

   These are operator equations. After some algebra, we get

   $$\partial_0\hat{\phi}(\vec{x}, x_0) = \hat{\Pi}(\vec{x}, x_0) \tag{116}$$
   $$\partial_0\hat{\Pi}(\vec{x}, x_0) = \bigtriangledown^2\hat{\phi}(\vec{x}, x_0) - m^2\hat{\phi}(\vec{x}, x_0) \tag{117}$$
   $$\left(\Box + m^2\right)\hat{\phi}(x) = 0 \tag{118}$$

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

2. *Field Expansion*:
   Let us solve this equation by Fourier Transforms. Let us write $\hat{\phi}(x)$ in the form

   $$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3}\, \hat{\phi}(\vec{k}, x_0)\, e^{i\vec{k}\cdot\vec{x}} \tag{119}$$

   where $\hat{\phi}(\vec{k}, x_0)$ are the Fourier amplitudes of $\hat{\phi}(x)$. We now demand that the $\hat{\phi}(x)$ satisfies the KG equation we find that $\hat{\phi}(\vec{k}, x_0)$ should satisfy the condition

   $$\partial_0^2\hat{\phi}(\vec{k}, x_0) + (\vec{k}^2 + m^2)\hat{\phi}(\vec{k}, x_0) = 0 \tag{120}$$

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

   $$\hat{\phi}^\dagger(\vec{k}, x_0) = \hat{\phi}(-\vec{k}, x_0) \tag{121}$$

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

$$\hat{\phi}(\vec{k}, x_0) = \hat{\phi}_+(\vec{k}) e^{i\omega(\vec{k})x_0} + \hat{\phi}_-(\vec{k}) e^{-i\omega(\vec{k})x_0} \tag{122}$$

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

$$\hat{\phi}_+(\vec{k}) = \hat{\phi}_-^\dagger(-\vec{k}) \qquad \hat{\phi}_+^\dagger(\vec{k}) = \hat{\phi}_-(-\vec{k}) \tag{123}$$

This expansion is a solution of the equations of motion if $\omega(\vec{k})$ is given by

$$\omega(\vec{k}) = \sqrt{\vec{k}^2 + m^2} \tag{124}$$

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

$$\hat{a}(\vec{k}) = 2\omega(\vec{k})\hat{\phi}_-(\vec{k}) \qquad \hat{a}^\dagger(\vec{k}) = 2\omega(\vec{k})\hat{\phi}_-^\dagger(\vec{k}) \tag{125}$$

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

$$[\hat{a}(\vec{k}), \hat{a}^\dagger(\vec{k}')] = (2\pi)^3 2\omega(\vec{k})\ \delta^3(\vec{k} - \vec{k}') \tag{126}$$

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

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \left[\hat{a}(\vec{k}) e^{-i\omega(\vec{k})x_0 + i\vec{k}\cdot\vec{x}} + \hat{a}^\dagger(\vec{k}) e^{i\omega(\vec{k})x_0 - i\vec{k}\cdot\vec{x}}\right] \tag{127}$$

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

The canonical momentum also can be expanded in a similar way

$$\hat{\Pi}(x) = -i \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \omega(k) [\hat{a}(\vec{k}) e^{-i\omega(\vec{k})x_0 + i\vec{k}\cdot\vec{x}} - \hat{a}^\dagger(\vec{k}) e^{i\omega(\vec{k})} e^{i\omega(\vec{k})x_0 - i\vec{k}\cdot\vec{x}}] \tag{128}$$

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

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \tag{129}$$

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.

3. *Hamiltonian*:
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 $\hat{a}(\vec{k})$ and $\hat{a}^\dagger(\vec{k})$. The result is

$$H = \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \frac{\omega(\vec{k})}{2} \left(\hat{a}(\vec{k})\hat{a}^\dagger(\vec{k}) + \hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) \right) \tag{130}$$

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

4. *Ground State*:
Let $|0\rangle$ be state which is anihilated by all the operators $\hat{a}(\vec{k})$, *i.e.,*

$$\hat{a}(\vec{k})|0\rangle = 0 \tag{131}$$

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

$$\hat{H} =: \hat{H} : + E_0 \tag{132}$$

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 $:\hat{H}:$ anihilates the vacuum

$$:\hat{H}: |0\rangle = 0 \tag{133}$$

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

$$E_0 = \int d^3k \frac{\omega(\vec{k})}{2} \delta(0) \tag{134}$$

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

$$\delta(0) = \lim_{p \to 0} \delta^3(\vec{p}) = \lim_{p \to 0} \int \frac{d^3x}{(2\pi)^3}\, e^{i\vec{p}\cdot\vec{x}} = \frac{V}{(2\pi)^3} \tag{135}$$

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

$$\varepsilon_0 = \int \frac{d^3k}{(2\pi)^3} \frac{\omega(\vec{k})}{2} \equiv \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \sqrt{\vec{k}^2 + m^2} \tag{136}$$

5. *Divergence*:

Eq. 136 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

$$\varepsilon_0 = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{\hbar\omega(k)}{2} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{1}{2} \sqrt{\frac{\hbar^2 K}{M} + \frac{4D\hbar^2}{M} \sin^2(\frac{ka}{2})} \tag{137}$$

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 *cut off* by the lattice spacing. However, the scalar field theory that we are considering does not have a cut off 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 cut off. The theory is now finite but one is left with the task of proving that the physics is independent of the cut off. This is the program of the Renormalization group. Although it is not presently known if there should be a fundamental cut off in these theories, *i.e.,* if there is a more fundamental description of Nature at short distances and high energies, it is clear that if these theories are to be regarded as effective *hydrodynamic* theories valid below some high energy scale, then a cut off is actually natural.

6. *Hilbert Space*:

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

$$:\hat{H}:= \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})}\ \omega(\vec{k})\ \hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) \tag{138}$$

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

$$\vec{P} = \int_{x_0 \text{ fixed}} d^3x\ \hat{\Pi}(\vec{x}, x_0)\vec{\bigtriangledown}\hat{\phi}(\vec{x}, x_0) \tag{139}$$

which, up to operator ordering amibiguities, is the quantum mechanical version of the classical linear momentum P^j,

$$P^j = \int_{x_0} d^3x\ T^{0j} \equiv \int_{x_0} d^3x\ \Pi(\vec{x}, x_0)\ \bigtriangledown^j\ \phi(\vec{x}, x_0) \tag{140}$$

In Fourier space $\vec{P}$ becomes

$$\vec{P} = \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \vec{k}\ \hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) \tag{141}$$

$\vec{P}$ has an operator ordering ambiguity which we will fix below by normal ordering. By inspection we see that $\vec{P}$ commutes with H.

$:\hat{H}:$ also commutes with the oscillator occupation number $\hat{n}(\vec{k})$, defined by

$$\hat{n}(\vec{k}) \equiv \hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) \tag{142}$$

Since $\{\hat{n}(\vec{k})\}$ and $\hat{H}$ commute with each other, we can use a complete set of eigenstates of $\{\hat{n}(\vec{k})\}$ to span the Hilbert space. Since we will regard the excitations counted by $\hat{n}(k)$ as *particles*, this Hilbert space has an indefinite number of particles and it is called *Fock space*. The states $\{|\{n(\vec{k})\}\rangle\}$, defined by

$$|\{n(\vec{k}\}\rangle = \prod_{\vec{k}} \mathcal{N}(\vec{k})[\hat{a}^\dagger(\vec{k})]^{n(\vec{k})}|0\rangle \tag{143}$$

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

$$\hat{n}(\vec{k})|\{n(\vec{k})\} >= (2\pi)^3 2\omega(\vec{k})n(\vec{k})|\{n(\vec{k}) > \tag{144}$$

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

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

$$\hat{N} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})}\hat{n}(\vec{k}) \tag{145}$$

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

$$\hat{N}|\{n(\vec{k})\}\rangle = \int d^3k\ n(\vec{k})\ |\{n(\vec{k})\}\rangle \tag{146}$$

The energy of these states is

$$\hat{H}|\{n(\vec{k})\}\rangle = \left[\int d^3k\ n(\vec{k})\omega(\vec{k}) + E_0\right]\ |\{n(\vec{k})\}\rangle \tag{147}$$

Thus, the *excitation energy* $\varepsilon(\{n(\vec{k})\})$ of this state is $\int d^3k\ n(\vec{k})\omega(\vec{k})$.

The operator $\vec{P}$ has an operator ordering ambiguity. It will be fixed by requiring that the vacuum state $|0\rangle$ be translationally invariant, *i.e.,* $\hat{P}^j|0\rangle = 0$. In terms of creation and anihilation operators we get

$$\hat{P}^j = \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} k^j \hat{n}(\vec{k}) \tag{148}$$

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

$$\hat{P}^j|\{n(\vec{k})\}\rangle = \left[\int d^3k\ k^j n(\vec{k})\right] |\{n(\vec{k})\}\rangle \tag{149}$$

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

The state $|\vec{k}\rangle$, defined by

$$|\vec{k}\rangle \equiv \hat{a}^\dagger(\vec{k})|0\rangle \tag{150}$$

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

$$E = \sqrt{\vec{k}^2 + m^2} \tag{151}$$

which is characteristic of a relativisitc *particle* of momentum $\vec{k}$ 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.

7. *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 spacial locations *commute* at equal times. But, do they commute at different times?

Let us calculate the commutator $\Delta(x-y)$

$$i\Delta(x-y) = [\hat{\phi}(x), \hat{\phi}(y)] \tag{152}$$

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

$$\hat{\phi}(x) = \hat{\phi}_+(x) + \hat{\phi}_-(x) \tag{153}$$

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

$$\begin{aligned} i\Delta(x-y) \qquad &= [\hat{\phi}_+(x), \hat{\phi}_+(y)] + [\hat{\phi}_-(x), \hat{\phi}_-(y)] \\ &+ [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] \end{aligned} \tag{154}$$

The first two terms always vanish since the $\hat{\phi}_+$ operators commute among themselves and so do the operators $\hat{\phi}_-$. Thus, we get

$$\begin{aligned} &i\Delta(x-y) = [\hat{\phi}_+(x), \hat{\phi}_-(y)] + [\hat{\phi}_-(x), \hat{\phi}_+(y)] = \\ &= \int d\bar{k} \int d\bar{k}' \{ [\hat{a}^\dagger(\vec{k}), \hat{a}(\vec{k}')] \; \exp\left(-i\omega(k)x_0 + i\vec{k}\cdot\vec{x} + i\omega(k')y_0 - i\vec{k}'\cdot\vec{y} \right) \\ &\quad + [\hat{a}(\vec{k}), \hat{a}^\dagger(\vec{k}')] \exp\left(i\omega(k)x_0 - i\vec{k}\cdot\vec{x} - i\omega(k'), y_0 + i\vec{k}'\cdot\vec{y} \right) \} \end{aligned} \tag{155}$$

where

$$\int d\bar{k} \equiv \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \tag{156}$$

By using the commutation relations, we get

$$i\Delta(x-y) = \int d\bar{k} \; [e^{i\omega(\vec{k})(x_0-y_0) - i\vec{k}\cdot(\vec{x}-\vec{y})} - e^{-i\omega(\vec{k})(x_0-y_0) + i\vec{k}\cdot(\vec{x}-\vec{y})}] \tag{157}$$

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

$$\epsilon(k^0) = \frac{k^0}{|k^0|} \equiv \text{sign}(k^0) \tag{158}$$

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

$$i\Delta(x-y) = \int \frac{d^4k}{(2\pi)^3} \delta(k^2 - m^2) \epsilon(k^0) e^{-ik\cdot(x-y)} \tag{159}$$

The integrand vanishes unless the *mass shell condition* $k^2 - m^2 = 0$ is satisfied. Notice that $\Delta(x-y)$ satisfies the initial condition

$$\partial_0 \Delta|_{x_0=y_0} = -\delta^3(\vec{x} - \vec{y}) \tag{160}$$

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

$$\Delta(\vec{x}-\vec{y},0) = 0 \tag{161}$$

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 $(x-y)^2 = (x_0-y_0)^2-(\vec{x}-\vec{y})^2 = (\vec{x}-\vec{y}^2)^2 < 0$, 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.

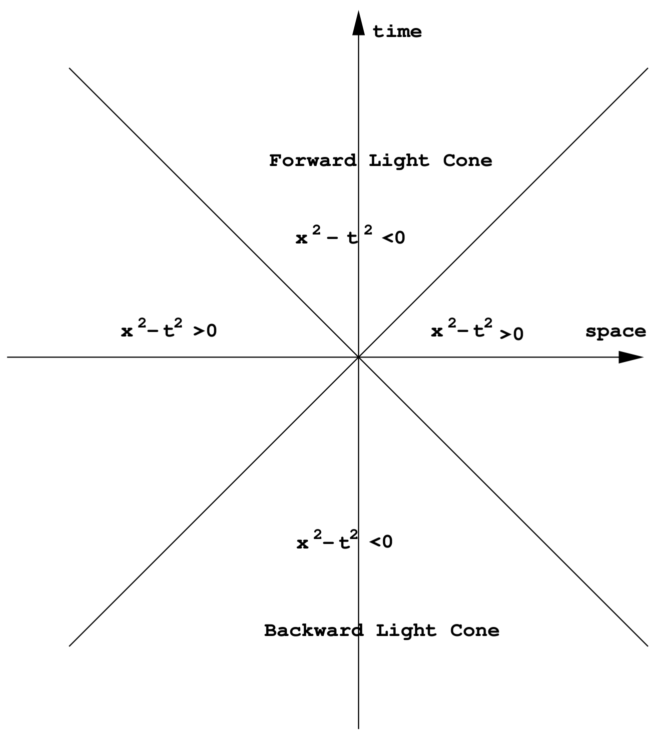

Figure 3: The light-cone.

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 which act on the Hilbert space of states. The classical statement that a quantity A is conserved if its Poisson Bracket with the Hamiltonian is zero

$$\frac{dA}{dt} = \{A, H\}_{PB} \tag{162}$$

becomes, in the quantum theory

$$i\frac{d\hat{A}_H}{dt} = [\hat{A}_H, \hat{H}] \tag{163}$$

and it applies to all operators in the Heisenberg representation. Then, the constants of motion of the quantum theory are operators which commute with the Hamiltonian.

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,

$$\hat{Q} = \int_{x_0 \text{ fixed}} d^3x \; \hat{j}^0(\vec{x}, x_0) \tag{164}$$

commutes with $\hat{H}$

$$[\hat{Q}, \hat{H}] = 0 \tag{165}$$

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

$$U(\alpha) = \exp(i\alpha\hat{Q}) \tag{166}$$

are unitary transformations which act on the Hilbert space of the theory.

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

$$P^\mu = \int_{x_0} d^3x \; T^{0\mu} \tag{167}$$

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

$$\{\phi(\vec{x}, x_0), P^j\}_{PB} = \partial_x^j \phi \tag{168}$$

In the quantum theory the equivalent statement is that the operators $\hat{\phi}(x)$ and $\hat{P}^j$ satisfy the equal-time commutation relation

$$[\hat{\phi}(x, x_0), \hat{P}^j] = i\partial_x^j \hat{\phi}(\vec{x}, x_0) \tag{169}$$

Consequently, $\hat{\phi}(x^j + a^j, x_0)$ and $\hat{\phi}(x^j, x_0)$ are related by

$$\hat{\phi}(x^j + a^j, x_0) = e^{ia_j \hat{P}_j} \hat{\phi}(\vec{x}, x_0) e^{-ia_j \hat{P}_j} \tag{170}$$

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

$$e^{ia_j \hat{P}^j}|0\rangle = |0\rangle \tag{171}$$

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 that we can consider is the *free complex scalar field* $\phi(x)$ whose Lagrangian $\mathcal{L}$ is invariant under global phase transformations. If ϕ is a complex field, we can decompose it into its real and imaginary parts

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \tag{172}$$

The Classical Lagrangian for a free complex scalar field ϕ is

$$\mathcal{L} = \partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi \tag{173}$$

now splits into two independent terms

$$\mathcal{L}(\phi) = \mathcal{L}(\phi_1) + \mathcal{L}(\phi_2) \tag{174}$$

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

$$\Pi(x) = \frac{\delta \mathcal{L}}{\delta \partial_0 \phi} = \frac{1}{\sqrt{2}}(\dot{\phi}_1 - i\dot{\phi}_2) \qquad \Pi^*(x) = \frac{1}{\sqrt{2}}(\dot{\phi}_1 + i\dot{\phi}_2) \tag{175}$$

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

$$[\hat{\phi}(\vec{x}, x_0), \hat{\Pi}(\vec{y}, x_0)] = i\delta^3(\vec{x} - \vec{y}) \tag{176}$$

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

$$\begin{aligned}
\hat{a}(\vec{k}) &= \frac{1}{\sqrt{2}} \left(\hat{a}_1(\vec{k}) + i\hat{a}_2(\vec{k}) \right) \\
\hat{a}^\dagger(\vec{k}) &= \frac{1}{\sqrt{2}} \left(\hat{a}_1^\dagger(k) - i\hat{a}_2^\dagger(\vec{k}) \right) \\
\hat{b}(\vec{k}) &= \frac{1}{\sqrt{2}} \left(\hat{a}_1(\vec{k}) - i\hat{a}_2(\vec{k}) \right) \\
\hat{b}^\dagger(\vec{k}) &= \frac{1}{\sqrt{2}} \left(\hat{a}_1^\dagger(\vec{k}) + i\hat{a}_2^\dagger(\vec{k}) \right)
\end{aligned} \tag{177}$$

which satisfy the algebra

$$[\hat{a}(\vec{k}), \hat{a}^\dagger(\vec{k}')] = [\hat{b}(\vec{k}), \hat{b}^\dagger(\vec{k}')] = (2\pi)^3 2\omega(\vec{k})\ \delta^3(\vec{k} - \vec{k}') \tag{178}$$

while all other commutators vanish. The Fourier expansion for the fields now is

$$\begin{aligned} \hat{\phi}(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \left(\hat{a}(\vec{k}) e^{-ik\cdot x} + \hat{b}^\dagger(\vec{k}) e^{ik\cdot x} \right) \\ \hat{\phi}^\dagger(x) &= \int \frac{d^3k}{(2\pi)^3 2\omega(k)} \left(\hat{b}(k) e^{-ik\cdot x} + \hat{a}^\dagger(k) e^{ik\cdot x} \right) \end{aligned} \tag{179}$$

where $\omega(\vec{k}) = \sqrt{\vec{k}^2 + m^2}$ and $k_0 = \omega(\vec{k})$. The normal ordered Hamiltonian is

$$:\hat{H}:= \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \omega(\vec{k}) \left(\hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) + \hat{b}^\dagger(\vec{k})\hat{b}(\vec{k}) \right) \tag{180}$$

and the total momentum $\hat{P}$ is

$$\hat{P}^j = \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} k^j \left(\hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) + \hat{b}^\dagger(\vec{k})\hat{b}(\vec{k}) \right) \tag{181}$$

we see that there are two types of quanta, a and b. The field ϕ creates b-quanta and it destroys a-quanta. The vacuum has no quanta.

The one-particle states have now a two-fold degeneracy since the states $\hat{a}^\dagger(\vec{k})|0\rangle$ and $\hat{b}^\dagger(\vec{k})|0\rangle$ have one particle of type a and one of type b respectively but these states have exactly the same energy, $\omega(\vec{k})$, and the same momentum $\vec{k}$. 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 which generates this symmetry? The classically conserved current is

$$j_\mu = i\phi^* \overleftrightarrow{\partial_\mu} \phi \tag{182}$$

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

$$\begin{aligned} \hat{Q} &= :\int d^3x\ i \left(\hat{\phi}^\dagger \partial_0 \hat{\phi} - \partial_0 \hat{\phi}^\dagger \hat{\phi} \right): \\ &= \int \frac{d^3k}{(2\pi)^3 2\omega(\vec{k})} \left(\hat{a}^\dagger(\vec{k})\hat{a}(\vec{k}) - \hat{b}^\dagger(\vec{k})\hat{b}(\vec{k}) \right) \\ &= \hat{N}_a - \hat{N}_b \end{aligned} \tag{183}$$

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 non-interacting case that we are discussing here, provided that $[\hat{Q}, \hat{H}] = 0$. Thus, although $\hat{N}_a$ and $\hat{N}_b$ may not be conserved *separately* in the general case, 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. The vacuum state has $N_a = N_b = 0$. Thus, the generator $\hat{Q}$ anihilates the vacuum

$$\hat{Q}|0\rangle = 0 \tag{184}$$

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

$$|0\rangle' = e^{i\hat{Q}\alpha}|0\rangle = |0\rangle \tag{185}$$

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.

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

$$|+, \vec{k}\rangle = \hat{a}^\dagger(\vec{k})\ |0\rangle \qquad |-, \vec{k}\rangle = \hat{b}^\dagger(\vec{k})\ |0\rangle \tag{186}$$

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

$$\begin{aligned} \hat{Q}|+, \vec{k}\rangle \qquad &= (\hat{N}_a - \hat{N}_b)\hat{a}^\dagger(\vec{k})|0>= \hat{N}_a\ \hat{a}^\dagger(\vec{k})|0\rangle = +|+, \vec{k}\rangle \\ \hat{Q}|-, \vec{k}\rangle \qquad &= (\hat{N}_a - \hat{N}_b)\ \hat{b}^\dagger(\vec{k})|0\rangle = -|-, \vec{k}\rangle \end{aligned} \tag{187}$$

Hence

$$\hat{Q}|\sigma, \vec{k}\rangle = \sigma\ |\sigma, \vec{k}\rangle \tag{188}$$

where $\sigma = \pm 1$. Thus, the state $\hat{a}^\dagger(\vec{k})|0\rangle$ has *positive* charge while $\hat{b}^\dagger(\vec{k})|0\rangle$ has *negative* charge. Under a finite transformation $U(\alpha) = \exp(i\alpha\hat{Q})$ they transform like

$$\begin{aligned} |+, \vec{k}\rangle' = U(\alpha)\ |+, \vec{k}\rangle \qquad &= \exp(i\alpha\hat{Q})\ |+, \vec{k}\rangle = e^{i\alpha}\ |+, \vec{k}\rangle \\ |-, \vec{k}\rangle' = U(\alpha)\ |-, \vec{k}\rangle \qquad &= \exp(i\alpha\hat{Q})|-, \vec{k}\rangle = e^{-i\alpha}\ |-, \vec{k}\rangle \end{aligned} \tag{189}$$

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

$$\hat{\phi}'(x) = \exp(-i\alpha\hat{Q})\ \hat{\phi}(x)\ \exp(i\alpha\hat{Q}) = e^{i\alpha}\hat{\phi}(x) \tag{190}$$

since

$$[\hat{Q}, \hat{\phi}(x)] = -\hat{\phi}(x) \qquad [\hat{Q}, \hat{\phi}^\dagger(x)] = \hat{\phi}^\dagger(x) \tag{191}$$

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 anihilate* particles of type a (which carry *positive* charge). The states $|\pm, \vec{k}\rangle$ are commonly referred to as *particles* and *antiparticles*: particles have rest mass m, momentum $\vec{k}$ 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 tell us that the states of the spectrum of the theory must transform like 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. However, there are many systems in Nature, such as magnets 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.