Hoofdstuk 1

Free quantum fields

1.1 What is a quantum field? What is a particle?

Consider a system with many degrees of freedom such as a glass of water, a crystal or a piece of string. If we are only interested in phenomena at a scale (space or time) much larger then the typical atomic or microscopic scales involved (distance between atoms in crystal or water, period of vibration of atom around equilibrum position etc ...) we can go over to a continuous description in terms of fields. For a vibrating string this field is the displacement field $q(x,t)$ which obeys the wave equation

$$\frac{1}{v^2}\frac{\partial^2 q}{\partial t^2} - \frac{\partial^2 q}{\partial x^2} = 0 \tag{1.1}$$

with v the propagation velocity.

When this system, which we approximately describe at these large scales with continuum fields, has quantum mechanical behavior, we should replace the fields by quantum fields ($q(x,t) \to \hat{q}(x,t)$) which obeys the same wave equation in the Heisenberg picture. Now we can use the uncertainty principle to replace space-time scales with momentum-energy scales:

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{1.2}$$

$$\Delta t \Delta E \geq \hbar \, . \tag{1.3}$$

From this we see that large space and time scales correspond to small momentum and energy scales. From this it follows that quantum field theorycan be used to describe the quantum mechanical behavior of systems with many degrees of freedom at energies and momenta much smaller then the typical “microscopic” energy and momentum scale. For energies larger then some cutoff scale(close to the microscopic scale) thecontinuous description is not valed anymore and the original microscopic variables have to be reintroduced.

Quantumfield theory can also be used if one does not know the “microscopic “ theory. Take for example Maxwell’s theory, Q.E.D. Here we only have the field theory, we have no fundamental "microscopic" theory for which the Maxwell theory is a low energetic approximation. At energies around 100 GeV this theory gets unified with weak interactions into the standard model for electro-weak interactions, the Weinberg-Salam model which is itself a low energetic field theoretic model of an even more fundamental theory which explains the many parameters of the Standard Model and is still not known (string theory?).

Finally there is the question: what is a particle. Why is the particle concept so useful and so omnipresent in modern physics? The answer is very general. Every system with many degrees of freedom can be described at low energy by a quantum field theory. Because of quantization, the low energy excitations of a quantum field theory behave as point particles without internal structure. We will illustrate this with a well known example: the vibrations in a crystal. But before we discuss the quantization of lattice vibrations, we will introduce canonical quantization, which is simply quantization in the Heisenberg picture.

1.2 Canonical quantization of a system with a finite number of degrees of freedom.

Newton's equations can be deduced from the principle of minimal action. For a system with one degree of freedom we have the Lagrangean:

$$L = \frac{1}{2} m \dot{q}^2 - V(q) \tag{1.4}$$

where$q$ can be the position of a particle and $V(q)$ its potential energy. De action is:

$$S = \int_{t_1}^{t_2} L(q, \dot{q}) dt \ . \tag{1.5}$$

We vary over all paths $q(t)$ that start in q_1 at $t = t_1$ and end in q_2 at $t = t_2$.The classical path is the one which minimizes the action:

$$\delta S = 0 \tag{1.6}$$

or

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) \\ &= \int_{t_1}^{t_2} dt \left(\delta q \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right] + \frac{d}{dt} \left(\delta q \frac{\partial L}{\partial \dot{q}} \right) \right) \\ &= \int_{t_1}^{t_2} dt \delta q \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right] = 0 \end{aligned} \tag{1.7}$$

where we used partial integration and the boundary conditions$\delta q(t_1) = \delta q(t_2) = 0$. Because the change in action for every variation δq has to be zero, we obtain the *Euler-Lagrangeequation:*

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0 \ . \tag{1.8}$$

This is the Lagrangian formalism. For quantization however, it is more appropriate to start from the Hamiltonian formalism. The Hamiltonian is defined as:

$$H(q,p) = p\dot{q} - L(q,\dot{q}) \tag{1.9}$$

where the *canonically conjugate momentum* p is defined as:

$$p = \frac{\partial L}{\partial \dot{q}} \ . \tag{1.10}$$

The transformation from the variables$q, \dot{q}$ to q, p is a so called Legendretransformation. Because

$$\begin{aligned} \delta H &= p\delta\dot{q} + \delta p\dot{q} - \frac{\partial L}{\partial q}\delta q - \frac{\partial L}{\partial \dot{q}}\delta\dot{q} \\ &= \dot{q}\delta p - \frac{\partial L}{\partial q}\delta q \\ &= \frac{\partial H}{\partial q}\delta q + \frac{\partial H}{\partial p}\delta p \end{aligned} \tag{1.11}$$

we find the Hamiltonian equations:

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q} \ . \tag{1.12}$$

The total derivative with respect to time of a physcial quantity $F(q,p)$ is:

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial p}\dot{p} \\ &= \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial H}{\partial q} \\ &= \frac{\partial F}{\partial t} + \{H, F\}_{PB} \end{aligned} \tag{1.13}$$

where the Poisson bracket is defined as:

$$\{A, B\}_{PB} = \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} - \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} \ . \tag{1.14}$$

We can now go from classical to quantum mechanics by the replacement:

$$\{A, B\}_{PB} \rightarrow \frac{i}{\hbar}[\hat{A}, \hat{B}] \ . \tag{1.15}$$

For canonically conjugate coordinates we find the canonical commutation relation:

$$[\hat{p}, \hat{q}] = -i\hbar \tag{1.16}$$

which can be realised in the configuration representation as:

$$\hat{p} \to -i\hbar \frac{\partial}{\partial q} \ , \qquad \hat{q} \to q \ . \tag{1.17}$$

The Hamiltonian equations of motion then become the well known equations of motion in the Heisnberg picture:

$$\dot{\hat{q}} = \frac{i}{\hbar}[\hat{H}, \hat{q}] \ , \qquad \dot{\hat{p}} = \frac{i}{\hbar}[\hat{H}, \hat{p}] \ . \tag{1.18}$$

This can be generalized to a system with N degrees of freedom. Let's take N particles with mass m connected by springs :

$$\begin{aligned} L &= \sum_{i=1}^{N} L_i \\ &= \sum_{i=1}^{N} \left[\frac{1}{2} m \dot{q}_i^2 - \frac{1}{2} \kappa (q_i - q_{i+1})^2 \right] \ . \end{aligned} \tag{1.19}$$

The Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{1.20}$$

give

$$m \ddot{q}_i = \kappa (q_{i-1} - 2q_i + q_{i+1}) \ . \tag{1.21}$$

The Hamiltonian becomes:

$$H = \sum_i p_i \dot{q}_i - L_i \tag{1.22}$$

with $p_i = \partial L / \partial \dot{q}_i = m \dot{q}_i$, and we can quantize through the canonical commutation relations:

$$[\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0 \tag{1.23}$$

$$[\hat{p}_i, \hat{q}_j] = -i\hbar \delta_{ij} \ . \tag{1.24}$$

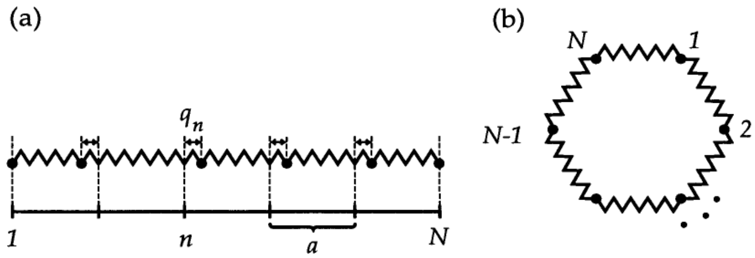
1.3 The linear crystal: classically.

Consider a linear crystal consisting of N atoms connected by elastic springs:

$$L = \sum_{i=-N/2}^{N/2} \left(\frac{m}{2} \dot{q}_i^2 - \frac{\kappa}{2} (q_i - q_{i+1})^2 \right) \ . \tag{1.25}$$

We impose periodic boundary conditions:

$$q_{N+1} = q_1 \tag{1.26}$$



Figuur 1.1: **(a)** A linear crystal composed of point particles **(b)** The linear crystal with periodic boundary conditions

(see figure1.1). The coordinate $q_i(t)$ describes the displacement of the i-th atom with respect to the equilibrum lattice. We limit ourselves to small vibrations (low energy) so that we can neglect anharmonic effects. The constant κ can be calculated from the microscopic theory of the crystal or can be measured experimentally. The Euler-Lagrange equation is

$$m\ddot{q}_i = \kappa(q_{i-1} - 2q_i + q_{i+1}) \ . \tag{1.27}$$

Let a be the lattice parameter so that:

$$q_i(t) = q(ia, t) = q(x, t) \tag{1.28}$$

In the limit $a \to 0$, $N \to \infty$ with $L = Na$ fixed, we have:

$$\frac{q_{i-1} - 2q_i + q_{i+1}}{a^2} \to \frac{\partial^2 q}{\partial x^2}(x, t) \ , \tag{1.29}$$

and we recover the wave equation

$$\left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) q(x, t) = 0 \tag{1.30}$$

for the displacement field $q(x, t)$ with

$$v = \sqrt{\frac{a^2 \kappa}{m}} \ . \tag{1.31}$$

The discrete equations (1.27) are coupled:

$$m\ddot{q} = \kappa A q \tag{1.32}$$

where theq_i have been put in aN-dimensional vector and A

$$A = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \sim a^2 \frac{\partial^2}{\partial x^2} \tag{1.33}$$

is a tridiagonal matrix.

These equations can be decoupled through the normal coordinates $c_k(t)$:

$$q_i(t) = \sum_k c_k(t) u_i^k \tag{1.34}$$

where the vectors $\{u^k\}$ form a basis which diagonalizes A. Because $A \sim a^2\partial^2/\partial x^2$ in the continuum limit and the operator $\partial^2/\partial x^2$ is diagonalized by the vectors $u^k = \frac{1}{\sqrt{2\pi}} e^{ikx}$, we propose as discrete version of the u^k:

$$u_i^k = \frac{1}{\sqrt{N}} e^{ikai} \ . \tag{1.35}$$

Indeed:

$$\begin{aligned}(Au^k)_i &= \frac{1}{\sqrt{N}}(e^{ika(i-1)} - 2e^{ikai} + e^{ika(i+1)}) \\ &= \frac{1}{\sqrt{N}} e^{ikai}(e^{ika} + e^{-ika} - 2) \\ &= 2(\cos ka - 1) u_i^k \ . \end{aligned} \tag{1.36}$$

Because the periodic boundary conditions have to be fulfilled we have:

$$k = \frac{2\pi}{Na} l \tag{1.37}$$

with l a whole number so that

$$-\frac{N}{2} < l \leq \frac{N}{2} \ . \tag{1.38}$$

By introducing normal coordinates we have decomposed the displacementet $q(t)$ in normal modes. k is nothing else than the wave vector for plane waves. For low momenta ($ka \ll \pi$) the eigenvalues of A are reduced to

$$2(\cos ka - 1) \rightarrow -k^2 a^2 \tag{1.39}$$

what can be expected because in the continuum limit (low momenta) $A \sim a^2\partial^2/\partial x^2$.

One can easily check that (excercise) the normal modes are orthonormal:

$$\langle k'|k\rangle = \sum_{i=1}^{N} u_i^{k'^*} u_i^k = \delta_{kk'} \tag{1.40}$$

with $\langle i|k\rangle = u_i^k$ the component of u^k along the i-th basis vector (the position of the i-th atom), and that they form an orthonormal basis of the N-dimensional configuration space (de position space of N atoms along the x-axis:

$$\sum_k \langle i'|k\rangle\langle k|i\rangle = \sum_k u_{i'}^{k^*} u_i^k = \delta_{i'i} \tag{1.41}$$

or the completeness relation:

$$\sum_k |k\rangle\langle k| = \mathbb{1}_{N\times N} \ . \tag{1.42}$$

Finally we thave that

$$u_i^{k*} = u_i^{-k} \tag{1.43}$$

so that , because the displacements are real

$$c_k^*(t) = c_{-k}(t) \ . \tag{1.44}$$

Projecting the equations of motion (1.27) on the k-th mode, we obtain:

$$\ddot{c}_k(t) = -\omega_k^2 c_k(t) \tag{1.45}$$

with

$$\omega_k = \sqrt{\frac{2\kappa}{m}(1-\cos ka)} = 2\sqrt{\frac{\kappa}{m}}\left|\sin\frac{ka}{2}\right| \ . \tag{1.46}$$

In this way, we have reduced the problem of the linear crystal to N decoupled oscillators with frequency ω_k en wave vector k.

The general solution of (1.45) is

$$c_k(t) = b_k e^{-i\omega_k t} + b_{-k}^* e^{+i\omega_k t} \tag{1.47}$$

so thatt

$$q_i(t) = \sum_k \left(b_k e^{-i\omega_k t} u_i^k + b_k^* e^{i\omega_k t} u_i^{k*}\right) \tag{1.48}$$

where by the reality condition (1.44) is automatically fulfilled.

The dispersion relation (see figure 1.2)

$$\omega_k = 2\sqrt{\frac{\kappa}{m}}\left|\sin\frac{ka}{2}\right| \ , \qquad -\frac{\pi}{a} < k < \frac{\pi}{a} \tag{1.49}$$

is reduced for low energy or momentume ($ka \to 0$) to

$$\omega_k = \sqrt{\frac{a^2\kappa}{m}}k = vk \tag{1.50}$$

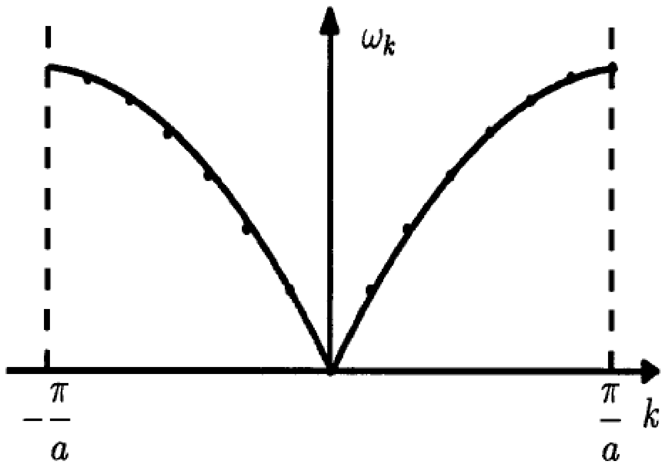
and theBrillouinzone $-\frac{\pi}{a} < k < \frac{\pi}{a}$ to$-\infty < k < \infty$.

1.4 Canonical quantization of the linear crystal.

To go from classical to quantum mechanics we replace the classical coordinates and momenta by linear operators $\hat{q}_i$ en $\hat{p}_i$ with commutation relations:

$$[\hat{q}_i, \hat{q}_j] = 0 \ , \qquad [\hat{p}_i, \hat{p}_j] = 0 \tag{1.51}$$

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij} \ . \tag{1.52}$$



Figuur 1.2: The dispersion relation of an oscillating chain . The points denote punten discrete values of k.

The quantum Hamiltonian is given by:

$$\hat{H} = \sum_{i=1}^{N} \frac{1}{2m}\hat{p}_i^2 + \sum_{i=1}^{N} \frac{\kappa}{2}(\hat{q}_{i+1} - \hat{q}_i)^2 \ . \tag{1.53}$$

The expansion coefficients b_k become linear operators$\hat{b}_k$,complex conjugation becomes Hermitean conjugation so that

$$\hat{q}_i(t) = \sum_k (\hat{b}_k(t)u_i^k + \hat{b}_k^\dagger(t)u_i^{k*}) \tag{1.54}$$

and

$$\hat{p}_i(t) = m\dot{\hat{q}}_i(t) = \sum_k (-im\omega_k)(\hat{b}_k(t)u_i^k - \hat{b}_k^\dagger(t)u_i^{k*}) \tag{1.55}$$

with $\hat{b}_k(t) = \hat{b}_k e^{-i\omega_k}$. From (1.54) and (1.55) it follows that

$$\frac{1}{2}\sum_i \left(\hat{q}_i(t) + \frac{i}{\omega_k m}\hat{p}_i(t)\right) u_i^{k*} = \hat{b}_k(t) \tag{1.56}$$

where we used the orthonormality relations of the basis vectors u^i_k. The commutation relations for the $\hat{b}$'s are:

$$\begin{aligned}
[\hat{b}_k, \hat{b}^\dagger_{k'}] &= \frac{1}{4}\sum_{i,j} u^{k^*}_i u^{k'}_j \left[\hat{q}_i + \frac{i}{\omega_k m}\hat{p}_i, \hat{q}_j - \frac{i}{\omega_{k'} m}\hat{p}_j\right] \\
&= \frac{1}{4}\sum_{i,j} u^{k^*}_i u^{k'}_j \left(\frac{i}{\omega_k m}[\hat{p}_i, \hat{q}_j] - \frac{i}{\omega_{k'} m}[\hat{q}_i, \hat{p}_j]\right) \\
&= \frac{1}{4}\frac{\hbar}{m}\sum_{i} u^{k^*}_i u^{k'}_i \left(\frac{1}{\omega_k} + \frac{1}{\omega_{k'}}\right) \\
&= \frac{\hbar}{2m\omega_k}\delta_{kk'} \qquad (1.57)
\end{aligned}$$

and

$$[\hat{b}_k, \hat{b}_{k'}] = 0 \ , \qquad [\hat{b}^\dagger_k, \hat{b}^\dagger_{k'}] = 0 \ . \qquad (1.58)$$

To streamline the formulas we go over to dimensionless operators $\hat{a}_k$, defined by

$$\hat{a}_k = \sqrt{\frac{2m\omega_k}{\hbar}}\hat{b}_k \qquad (1.59)$$

so that the mode expansions become:

$$\hat{q}_i(t) = \sum_k \sqrt{\frac{\hbar}{2m\omega_k}}(\hat{a}_k(t)u^k_i + \hat{a}^\dagger_k(t)u^{k^*}_i) \qquad (1.60)$$

$$\hat{p}_i(t) = -i\sum_k \sqrt{\frac{\hbar m\omega_k}{2}}(\hat{a}_k(t)u^k_i - \hat{a}^\dagger_k(t)u^{k^*}_i) \qquad (1.61)$$

and the commutation relations:

$$[\hat{a}_k, \hat{a}_{k'}] = 0 \ , \qquad [\hat{a}^\dagger_k, \hat{a}^\dagger_{k'}] = 0 \qquad (1.62)$$

$$[\hat{a}_k, \hat{a}^\dagger_{k'}] = \delta_{kk'} \ . \qquad (1.63)$$

The physical interpretation of the operators $\hat{a}_k$ en $\hat{a}^\dagger_k$ is straightforward. Because $\hat{a}_k(t) = e^{-i\omega_k t}\hat{a}_k$, we have in the Heisenberg picture:

$$i\hbar\frac{d}{dt}\hat{a}_k(t) = [\hat{a}_k(t), \hat{H}] = \hbar\omega_k\hat{a}_{k'} \qquad (1.64)$$

and hence

$$[\hat{H}, \hat{a}_k] = -\hbar\omega_k\hat{a}_k \ . \qquad (1.65)$$

If $|\psi\rangle$ is an eigenstate of $\hat{H}$ met energie E, then $a_k|\psi\rangle$ is an eigenstate of $\hat{H}$ with energy $E - \hbar\omega_k$. Indeed:

$$\begin{aligned}
\hat{H}\hat{a}_k|\psi\rangle &= [\hat{H}, \hat{a}_k]|\psi\rangle + \hat{a}_k\hat{H}|\psi\rangle \\
&= (E - \hbar\omega_k)\hat{a}_k|\psi\rangle \ . \qquad (1.66)
\end{aligned}$$

The operator $\hat{a}_k$ destroys a quantum with energy $\hbar\omega_k$. Therefor we call $\hat{a}_k$ an annihilation operator for a quantum with wave vector k . Analogously

$$[\hat{H}, \hat{a}_k^\dagger] = \hbar\omega_k \hat{a}_k^\dagger \tag{1.67}$$

and $\hat{a}_k^\dagger$ is a so called creation operator for a quantum of the mode with wave vector k. From the theory of the harmonic oscillator we know that the Hamiltonion can be written as:

$$\hat{H} = \sum_k \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \ . \tag{1.68}$$

Indeed, from the commutation relations follow (1.65) and (1.67). This also follows by careful calculation using the Hamiltonian (1.53), the expansions (1.54) and (1.55) and the orthonormality relations for the basis vectors u^k.

The groundstate $|\Theta\rangle$ of our crystal contains no quanta and hence is annihilated by all $\hat{a}_k$:

$$\hat{a}_k |\Theta\rangle = 0 \tag{1.69}$$

with $|\Theta\rangle = \prod_k |\Theta_k\rangle$, where $|\Theta_k\rangle$ is the groundstate of the k-th mode. Excited states can be obtained by applying the creators $\hat{a}_k^\dagger$:

$$|n\rangle = |n_1, n_2, \cdots\rangle = \prod_k |n_k\rangle \tag{1.70}$$

with for every mode:

$$|n_k\rangle = \frac{1}{\sqrt{n_k!}} (a_k^\dagger)^{n_k} |\Theta_k\rangle \ . \tag{1.71}$$

Introducing the number operator $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ which counts the number of quanta with energy $\hbar\omega_k$, we have

$$\hat{H} = \sum_k \hbar\omega_k \left(\hat{n}_k + \frac{1}{2} \right) \ . \tag{1.72}$$

The interpretation of (1.72) is now very simple. Every mode contributes $\hbar\omega_k/2$ (zero point energy) and for n_k quanta $n_k\hbar\omega_k$ to the total energy of the system . These quanta of vibration are well known in condensed matter physics and are called phonons. In realistic crystals with at least two atoms per unit cell, there are two types of phonons : optical and acoustic phonons . The phonons which we discuss here are acoustic and low energy or long wave length phonons generate sound in crystals.With a phonon with wave vector k we can associate a crystal momentum $p = \hbar k$ which behaves as a real momentum and is conserved in phonon scattering or phonon creation modulo a vector of the reciprocal lattice. (This is so because continuous translational symmetry is broken to the discrete translational symmetry of the lattice) These phonons have a bosonic character.This is a direct consequence of the commutation relations. Suppose we have two phonons with wave vector k_1 en k_2 described by

$$|k_1, k_2\rangle = \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger |\Theta\rangle \ . \tag{1.73}$$

Because $[\hat{a}^\dagger_k, \hat{a}^\dagger_{k'}] = 0$, we have

$$|k_1, k_2\rangle = |k_2, k_1\rangle \tag{1.74}$$

so that these quanta behave as bosons.

1.5 Canonical quantization in the continuum limit.

In the first paragraph, we have defined quantum field theory as the quantum mechanics of a system with very many degrees of freedom in the low energy limit. The low energy excitations behave as point particles. Let us illustrate this now in the case of the linear crystal. The dispersion relation for the mode with wave number k is:

$$\begin{aligned} \omega_k &= 2\sqrt{\frac{\kappa}{m}}\left|\sin\frac{ka}{2}\right| , \qquad -\frac{\pi}{a} < k \leq \frac{\pi}{a} \\ &\sim v|k| , \quad |k| \ll \frac{\pi}{a} . \end{aligned} \tag{1.75}$$

If we introduce the crystal momentum $p = \hbar k$, then the excitation energy of the k-th mode:

$$\begin{aligned} E_p = \hbar\omega_k &= v\hbar|k| \\ &= v|p| . \end{aligned} \tag{1.76}$$

Here v is the propagation velocity of sound in the crystal.

At low energy, only acoustic phonons and hence sound waves can be used to exchange messages or energy. Thus, v plays the role of the "velocity of light". If we interpret this analogy literally, then we can rewrite (**??**) as:

$$E_p = c|p| . \tag{1.77}$$

Now, the Einstein relation between energy and momentum of a particle with restmass $m_0$is:

$$E_p = \sqrt{m_0^2c^4 + c^2p^2} , \tag{1.78}$$

so that we can say that low energy excitations of the crystal (acoustic phonons) behave as point particles with zero mass.. Since at low energy there are only low energy acoustic phonons in a crystal we can say that the low energy physics of a crystal is equivalent to a massless scalar field theory.

We can show this equivalence also in another way. Let's look at the crystal with low spacial and temporal resolution. Then the image of the crystal lattice is blurred and the lattice can be viewed as an elastic continuum. We get the same image by letting the lattice parameter a go to zero so that the length of the crystal $L = Na$ remains constant or $N \sim 1/a \to \infty$. Mathematically this means that we go over from lattice sums to space integrals:

$$a\sum_i f_i = \sum_i af(ia) \to \int_{-L/2}^{L/2} f(x)dx . \tag{1.79}$$

The Kronecker-delta becomes a Dirac -deltafunction at low resolution:

$$
\begin{aligned}
& a \sum_i f(ia) \frac{1}{a} \delta_{ij} = f(ja) \\
\xrightarrow[a \to 0]{} & \int_{-L/2}^{L/2} f(x) \delta(x-y) dx = f(y) \ , \qquad (1.80)
\end{aligned}
$$

so that

$$
\frac{\delta_{ij}}{a} \to \delta(x-y) \ . \qquad (1.81)
$$

We can now rewrite the completenesss relations for the basis vectors u^k as:

$$
\frac{\delta_{ij}}{a} = \frac{1}{a} \sum_k u_j^{k*} u_i^k = \frac{1}{Na} \sum_{k=-\pi/a}^{\pi/a} e^{ika(i-j)} \ . \qquad (1.82)
$$

Because

$$
k = \frac{2\pi}{Na} l = \frac{2\pi}{L} l \ , \qquad -\frac{N}{2} < l \leq \frac{N}{2} \qquad (1.83)
$$

and taking besides the limit $a \to 0$ also the limit $L \to 0$ (infinitely long crystal), the k-spectrum becomes continuous and the distance between to adjacent k-values

$$
\Delta k = \frac{2\pi}{Na} = \frac{2\pi}{L} \xrightarrow[L \to \infty]{} dk \qquad (1.84)
$$

becomes the differential dk. (1.82) can be rewritten in the limit $a \to 0$, $L \to \infty$ as

$$
\begin{aligned}
\delta(x-y) &= \lim_{\substack{a \to 0 \\ L \to \infty}} \frac{1}{2\pi} \sum_{k=-\pi/a}^{\pi/a} \Delta k \ e^{ika(i-j)} \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \ e^{ik(x-y)} \ , \qquad (1.85)
\end{aligned}
$$

what turns out to be the well known expression for the Dirac-deltafunction as a Fourier integral.

Let us turn back now to the linear crystal, then the Lagrangian becomes in de limit $a \to 0$, $L \to \infty$:

$$
\begin{aligned}
L &= a \left[\sum_{i=-N/2}^{N/2} \frac{m}{a} \dot{q}_i^2 - a\kappa \left(\frac{q_i - q_{i+1}}{a} \right)^2 \right] \\
&\underset{\substack{a \to 0 \\ L \to \infty}}{=} \int_{-\infty}^{+\infty} dx \ \frac{1}{2} \left[\rho \left(\frac{\partial q}{\partial t}(x,t) \right)^2 - Y \left(\frac{\partial q}{\partial x}(x,t) \right)^2 \right] \qquad (1.86)
\end{aligned}
$$

where$\rho = m/a$ is the mass density per unit of length , $Y = \kappa a$ the Young modulus and $q(x,t) = q_i(t)$ with $x = ia$. If we rescale the field q as

$$\phi = \sqrt{Y} q \ , \tag{1.87}$$

then it follows from

$$v = \sqrt{\frac{a^2 \kappa}{m}} = \sqrt{\frac{Y}{\rho}} \tag{1.88}$$

that

$$L = \int_{-\infty}^{+\infty} dx \ \frac{1}{2} \left[\frac{1}{v^2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \left(\frac{\partial \phi}{\partial x} \right)^2 \right] \ . \tag{1.89}$$

In the low energy limit or continuum limit we can write the Lagrangian of our linear crystal as the "volume"-integral of the Lagrangian density $\mathcal{L}$ with

$$\mathcal{L} = \frac{1}{2} \left[\frac{1}{v^2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \left(\frac{\partial \phi}{\partial x} \right)^2 \right] \ . \tag{1.90}$$

Introducing the "relativistic" notation:

$$\partial_\mu = \left(\frac{1}{v} \frac{\partial}{\partial t}, \frac{\partial}{\partial x} \right) \ , \tag{1.91}$$

then this Lagrangian density is a Lorentz scalar:

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi \ . \tag{1.92}$$

The action defined as

$$S = \int_{t_1}^{t_2} dt \ L \ , \tag{1.93}$$

can be rewritten as the integral over two dimensional space time continuum:

$$\begin{aligned} S &= \int_{t_1}^{t_2} dt \int_{-\infty}^{+\infty} dx \ \mathcal{L}(\phi, \partial_\mu \phi) \\ &= \frac{1}{v} \iint d^2x \ \mathcal{L}(\phi, \partial_\mu \phi) \end{aligned} \tag{1.94}$$

with $x_0 = vt$.

The Lagrangian density (1.92) is the one of a massless scalar Klein–Gordon field. So we recover the idea that the low energy excitations of a crystal are massless particles. The Lorentz invariance we find here is an example of a dynamical symmetry. This symmetry is dynamically realised at low energy and is no fundamental symmetry of the crystal Lagrangian. An important lesson to be learned from this example is that maybe the Lorentz

Invariance of our fundamental laws of physics can be dynamically realised and that the microscopic theory of our world at high energy maybe has no Lorentz Invariance.

We now try to construct a continuum version (low energy limit) of the Hamiltonian formalism for the linear crystal. From the commutation relations

$$[q_i(t), p_j(t)] = m[q_i(t), \dot{q}_j(t)] = i\hbar\delta_{ij} \tag{1.95}$$

with

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{1.96}$$

it follows because ofv$\phi = \sqrt{Y}q$, $\rho = m/a$ and $Y = \kappa a$ that:

$$i\hbar\frac{\delta_{ij}}{a} = \frac{\rho}{Y}[\phi(ia,t), \dot{\phi}(ja,t)] \ , \tag{1.97}$$

or in the limit $a \to 0$:

$$i\hbar\delta(x-y) = [\phi(x,t), \pi(y,t)] \tag{1.98}$$

with

$$\pi(x,t) = \frac{1}{v^2}\dot{\phi}(x,t) \ . \tag{1.99}$$

The field $\pi(x,t)$ is called the canonically conjugate field. Indeed, from the expression for the Lagrangian density (1.90) follows

$$\pi(x,t) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x,t)} = \frac{1}{v^2}\dot{\phi}(x,t) \ , \tag{1.100}$$

which is precisely the continuum version of the discrete

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \ . \tag{1.101}$$

The canonical commutation relation (1.98) is nothing else then the continuum version of

$$[q_i, p_j] = i\hbar\delta_{ij} \ . \tag{1.102}$$

The Hamiltonian

$$H = \sum_{i=-N/2}^{N/2} (p_i\dot{q}_i - L_i) \tag{1.103}$$

can be rewritten in the limit $a \to 0$, $L \to \infty$ in the continuum form:

$$H = \int_{-\infty}^{+\infty} dx \ \mathcal{H}(\phi, \pi) \tag{1.104}$$

with $\mathcal{H}(\phi, \pi)$ the Hamiltonian density defined by

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L} \ . \tag{1.105}$$

We can also tale the continuum limit for the commutation relations of creation and annihilation operators and $L \to \infty$. Precisely as

$$\frac{\delta_{ij}}{a} = \frac{\delta_{ij}}{\Delta x} \xrightarrow[a\to 0]{} \delta(x-y) \tag{1.106}$$

we have

$$\frac{\delta_{kk'}}{\Delta k} \xrightarrow[L\to\infty]{} \delta(k-k') \ . \tag{1.107}$$

Definining the creation and annihilation operators in the $a \to 0$, $L \to \infty$ limit as

$$a(k) = \frac{a_k}{(\Delta k)^{1/2}} \ , \qquad a^\dagger(k) = \frac{a_k^\dagger}{(\Delta k)^{1/2}} \ , \tag{1.108}$$

we find:

$$[a(k), a^\dagger(k')] \underset{\substack{a\to 0\\ L\to\infty}}{=} \delta(k-k') \ . \tag{1.109}$$

and

$$[a(k), a(k')] = [a^\dagger(k), a^\dagger(k')] = 0 \ . \tag{1.110}$$

Coming back to the mode expansion (1.60) of $\hat{q}_i(t)$:

$$\begin{aligned} \hat{q}_i(t) &= \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} (\hat{a}_k(t) u_i^k + \hat{a}_k^\dagger(t) u_i^{k*}) \\ &= \Delta k \sum_k \sqrt{\frac{\hbar}{2m\omega_k}} \left(\frac{\hat{a}_k(t)}{\Delta k} \frac{1}{\sqrt{N}} e^{ikia} + \text{h.c.} \right) \ . \end{aligned} \tag{1.111}$$

and multiplying these equations with $\sqrt{Y}$ and using $m = \rho a$, we obtain

$$\hat{\phi}(ia, t) = \sum_k \frac{\Delta k}{\sqrt{2\pi}} \sqrt{\frac{\hbar Y}{2\omega_k \rho}} \left(\frac{\hat{a}_k(t)}{\Delta k} \sqrt{\frac{2\pi}{Na}} e^{ikia} + \text{h.c.} \right) \ , \tag{1.112}$$

In the limit $a \to 0$, taking into account that $\Delta k = 2\pi/Na = 2\pi/L$ we find:

$$\hat{\phi}(x, t) = \sum_k \frac{\Delta k}{\sqrt{2\pi}} \sqrt{\frac{\hbar v^2}{2\omega_k}} \left(\frac{\hat{a}_k(t)}{(\Delta k)^{1/2}} e^{ikx} + \text{h.c.} \right) \ . \tag{1.113}$$

If we finally take the limit$L \to \infty$, then $\Delta k \to dk$ and we obtain

$$\hat{\phi}(x, t) = \int_{-\infty}^{+\infty} \frac{dk}{(2\pi)^{1/2}} \sqrt{\frac{\hbar v^2}{2\omega_k}} (\hat{a}(k, t) e^{ikx} + \text{h.c.}) \ . \tag{1.114}$$

We find an analogous expansion for $\hat{\pi}$ from$\pi = \frac{1}{v^2}\dot{\phi}$:

$$\hat{\pi}(x, t) = \frac{1}{v^2}(-i) \int_{-\infty}^{+\infty} \frac{dk}{(2\pi)^{1/2}} \sqrt{\frac{\hbar v^2}{2\omega_k}} (\hat{a}(k, t) e^{ikx} - \text{h.c.}) \ . \tag{1.115}$$

What we learned from the continuum limit of the linear crystal can be generalised to an arbitrary Lorentz invariant scalar quantum field theory (with or without microsocpic description) in D spacetime dimensions (D-1 space dimensions and one time dimension).We define the action as an integral over the hypervolume Ω of spacetime of the Lagrangian density$\mathcal{L}(\phi, \partial_\mu \phi)$

$$S = \int_\Omega d^D x \; \mathcal{L}(\phi, \partial_\mu \phi) \; . \tag{1.116}$$

The continuum version of the Euler-Lagrange equations is obtained by extremising S over ϕ where we keepϕconstant on the boundary $\partial\Omega$ of spacetime (generalisation of $\delta q_i(t_1) = \delta q_i(t_2) = 0$):

$$\begin{aligned} \delta S &= \int_\Omega d^D x \left(\frac{\partial \mathcal{L}}{\partial \phi} \delta\phi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta \partial_\mu \phi \right) \\ &= \int_\Omega d^D x \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right) \delta\phi + \int_\Omega d^D x \; \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta\phi \right) \; . \end{aligned} \tag{1.117}$$

Making use of the theorem of Gauss we find:

$$\int_\Omega d^D x \; \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta\phi \right) = \int_{\partial\Omega} dS_\mu \; \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta\phi = 0 \; , \tag{1.118}$$

because the variation of the field on the hypersurface $\partial\Omega$ which is the boudary of the spacetime volume$\Omega$is zero. Putting the variation of the action equal to zero for all variations $\delta\phi$, we find the Euler-Lagrange equations

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \; . \tag{1.119}$$

Using the Lagrangian density of the linear crystal (1.92) we find

$$\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = \partial^\mu \phi \; , \qquad \frac{\partial \mathcal{L}}{\partial \phi} = 0 \; , \tag{1.120}$$

so that the Euler Lagrange equations become:

$$\partial_\mu \partial^\mu \phi = \Box \phi = \left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) \phi = 0 \; . \tag{1.121}$$

The Hamiltonian obviously becomes

$$H = \int d^{D-1} x \; \mathcal{H} \tag{1.122}$$

with

$$\mathcal{H} = \pi \dot{\phi} - \mathcal{L} \tag{1.123}$$

and

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \ . \tag{1.124}$$

Finally, the canonical commutation relations are:

$$[\phi(\vec{x},t), \phi(\vec{y},t)] = [\pi(\vec{x},t), \pi(\vec{y},t)] = 0 \tag{1.125a}$$

$$[\phi(\vec{x},t), \pi(\vec{y},t)] = i\hbar\delta^{D-1}(\vec{x}-\vec{y}) \ . \tag{1.125b}$$

1.6 Canonical quantisaton of the Klein–Gordonfield.

If one wants to combine the principle of relativity with the postulates of quantum mechanics one naturally arrives at relativistic quantum field theory. The relativistic demand of finite propagation velocity of interactions can be simply realised in a Lorentz invariant local field theory where a local perturbation of the field can only influence the immediate neighbourhood and propagates with finite velocity. Starting from now, we will mainly study quantum field theory for its own sake without asking questions about the underlying microscopic theory. We will frequently work in units where waar $\hbar = 1$ en $c = 1$. These units are a standard choice in elementary particle physics and are called *natural units*. The real Klein–Gordonveld φ describes an uncharged scalar (spin 0) free particle with mass m and satisfies the field equation

$$(\Box + m^2)\varphi = 0 \tag{1.126}$$

with$\Box = \partial^2/\partial t^2 - \nabla^2$ the d'Alembertian. The Klein–Gordon equation can be derived from the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \varphi)^2 - \frac{m^2}{2}\varphi^2 \ . \tag{1.127}$$

The canonically conjugate field is:

$$\pi(\vec{x},t) = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}(\vec{x},t)} = \dot{\varphi}(\vec{x},t) \tag{1.128}$$

The energy and momentum carried by this field are conserved quantities as follows from the Noether theorem.

Noether'sTheorem for translations and energy momentum conservation

Let's consider a translation over a constant four vector a^μ

$$x^\mu \to x^\mu + a^\mu \ , \tag{1.129}$$

then the field φ transforms as:

$$\varphi(x) \to \varphi(x+a) = \varphi(x) + \delta\varphi(x) \tag{1.130}$$

with

$$\delta\varphi(x) = a^\mu \partial_\mu \varphi(x) \ . \tag{1.131}$$

The change of the Lagrangian which is only dependent on φ en $\partial_\mu\varphi$ and hence not explicitely dependent on space and time is given by:

$$\delta\mathcal{L} = a^\mu \partial_\mu \mathcal{L} = \frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi + \frac{\partial\mathcal{L}}{\partial\partial^\mu\varphi}\delta\partial^\mu\varphi \ . \tag{1.132}$$

Because

$$\delta\partial^\mu\varphi = \partial^\mu\delta\varphi = a^\nu\partial^\mu\partial_\nu\varphi \tag{1.133}$$

and the Euler-Lagrange equation (1.119), (1.132) becomes:

$$\begin{aligned}\delta\mathcal{L} = a^\mu\partial_\mu\mathcal{L} &= \partial^\mu\left(\frac{\partial\mathcal{L}}{\partial\partial^\mu\varphi}\right)a^\nu\partial_\nu\varphi + \frac{\partial\mathcal{L}}{\partial\partial^\mu\varphi}a^\nu\partial^\mu\partial_\nu\varphi \\ &= a^\nu\partial^\mu\left(\frac{\partial\mathcal{L}}{\partial\partial^\mu\varphi}\partial_\nu\varphi\right)\end{aligned} \tag{1.134}$$

or

$$a^\nu\partial^\mu T_{\mu\nu} = 0 \tag{1.135}$$

with

$$T_{\mu\nu} = -g_{\mu\nu}\mathcal{L} + \frac{\partial\mathcal{L}}{\partial\partial^\mu\varphi}\partial_\nu\varphi \ . \tag{1.136}$$

For arbitrary constant a^ν we obtain the conservation law

$$\partial^\mu T_{\mu\nu} = 0 \ . \tag{1.137}$$

Therefore, with every translational degree of freedom ν corresponds a conserved current

$$J_{\mu\nu} = T_{\mu\nu} \ . \tag{1.138}$$

Integrating this conservation law over a volume V with surface S, we obtain

$$\partial^0\int_V d^3x\ T_{0\nu} - \int_V d^3x\ \nabla_i T_{i\nu} = 0 \ . \tag{1.139}$$

Using Gauss's theorem:

$$\int_V d^3x\ \nabla_i T_{i\nu} = \oint_S dS_i\ T_{i\nu} \tag{1.140}$$

we can rewrite (1.139) as

$$\frac{d}{dt}\int_V d^3x\ T_{0\nu} = \oint_S dS_i\ T_{i\nu} \ . \tag{1.141}$$

If we take$\nu = j = 1,2,3$ and define P_j as the total momentum in the j-th direction containedin the volume V, then the formula

$$P_j = \int_V d^3x\ T_{0j} \Rightarrow \frac{d}{dt}P_j = \oint_S dS_i\ T_{ij} \tag{1.142}$$

states that the amount of j-momentum that escapes from the volume V per unit of time equals the amount of j-momentum that flows through the surface S . The tensor T_{ij} can thus be interpreted as the current J_{ij} of j-momentum along the i-th direction. If we take an infinite volume and assume that the fields die off fast enough at infinity, then the right hand side of (1.142) is zero, and we obtain conservation of momentum in the j-direction:

$$\frac{d}{dt} P_j = 0 \; . \tag{1.143}$$

We can repeat the same for$\nu = 0$ with

$$P_0 = \int d^3x \; T_{00} = E \tag{1.144}$$

and then (1.141) for an infinite volume gives us the law of conservation of energy. From Noether's theorem it follows that we can define the conserved energy momentum four vector as

$$P^\mu = \int d^3x \; T^{0\mu} \tag{1.145}$$

and the corresponding conserved currents are given by the energy momentum tensor $T_{\mu\nu}$ defined in (1.136).

To find the enenergy and momentum of the Klein–Gordonveld we use (1.136) and (1.127)

$$\begin{aligned} T^{00} &= \left(\frac{\partial\varphi}{\partial t}\right)^2 - \mathcal{L} \\ &= \frac{1}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2 + \frac{1}{2}(\vec{\nabla}\varphi)^2 + \frac{m^2}{2}\varphi^2 \\ &= \frac{1}{2}\pi^2 + \frac{1}{2}(\vec{\nabla}\varphi)^2 + \frac{m^2}{2}\varphi^2 \end{aligned} \tag{1.146}$$

and

$$T^{0i} = -\frac{\partial\varphi}{\partial t}\nabla_i\varphi = -\pi\nabla_i\varphi \; , \tag{1.147}$$

so that the energy or Hamiltonian is given by:

$$H = \int d^3x \; \frac{1}{2}\left(\pi^2 + (\vec{\nabla}\varphi)^2 + m^2\varphi^2\right) \tag{1.148}$$

and the momentum $\vec{P}$ by

$$\vec{P} = -\int d^3x \; \pi\vec{\nabla}\varphi \; . \tag{1.149}$$

To quantize the Klein–Gordon field, we promote the canonically conjugate fields $\varphi(\vec{x}, t)$ en $\pi(\vec{x}, t)$ to quantum field operators which in natural units obey:

$$[\varphi(\vec{x}, t), \varphi(\vec{y}, t)] = [\pi(\vec{x}, t), \pi(\vec{y}, t)] = 0 \tag{1.150a}$$

$$[\varphi(\vec{x}, t), \pi(\vec{y}, t)] = i\delta(\vec{x} - \vec{y}) \; . \tag{1.150b}$$

Our next task is to diagonalize the Hamiltonian. By transforming to momentum space

$$\varphi(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} \tilde{\varphi}(\vec{k},t) \tag{1.151}$$

(with$\tilde{\varphi}^\dagger(\vec{k}) = \tilde{\varphi}(-\vec{k})$ so that φ is real) the Klein–Gordon equation becomes:

$$\left[\frac{\partial^2}{\partial t^2} + \left(|\vec{k}|^2 + m^2\right)\right] \tilde{\varphi}(\vec{k},t) = 0 \ . \tag{1.152}$$

This is the same equation as a harmonic oscillator with

$$\omega(\vec{k}) = \sqrt{|\vec{k}|^2 + m^2} \ . \tag{1.153}$$

The Hamiltonian of the harmonic oscillator

$$H_{H.O.} = \frac{p^2}{2} + \frac{\omega^2}{2} q^2 \tag{1.154}$$

can be diagonalised by introducing annihilation and creation operators

$$q = \frac{1}{\sqrt{2\omega}}(a + a^\dagger) \ , \qquad p = (-i)\sqrt{\frac{\omega}{2}}(a - a^\dagger) \ . \tag{1.155}$$

One can easily check that the commutation relation $[q,p] = i$ is equivalent to

$$[a, a^\dagger] = 1 \ . \tag{1.156}$$

The Hamiltonian can now be written as

$$H_{\text{H.O.}} = \omega \left(a^\dagger a + \frac{1}{2}\right) \ . \tag{1.157}$$

The groundstate $|0\rangle$ defined by $a|0\rangle = 0$ is an eigenstate of H with eigenvalue $\omega/2$, the *zero point energy.* From the commutators:

$$[H_{\text{H.O.}}, a^\dagger] = \omega a^\dagger \ , \quad [H_{\text{H.O.}}, a] = -\omega a \tag{1.158}$$

it easily follows that

$$|n\rangle = (a^\dagger)^n |0\rangle \tag{1.159}$$

are eigenstates of $H_{\text{H.O.}}$ with eigenvalue $(n + \frac{1}{2})\omega$. These states form the spectrum.

We can determine the spectrum of the Klein–Gordon-Hamiltonian by using the same trick for every Fourier mode $\tilde{\varphi}(\vec{k},t)$ which can be viewed as an independent oscillator with creation and annihilation operators $a^\dagger(\vec{k})$ en $a(\vec{k})$. At $t = 0$, where Schrödinger and Heisenberg picture coincide, we have :

$$\varphi(\vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}} \left(a(\vec{k})e^{i\vec{k}\cdot\vec{x}} + a^\dagger(\vec{k})e^{-i\vec{k}\cdot\vec{x}}\right) \tag{1.160a}$$

$$\pi(\vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} (-i)\sqrt{\frac{\omega(k)}{2}} \left(a(\vec{k})e^{i\vec{k}\cdot\vec{x}} - a^\dagger(\vec{k})e^{-i\vec{k}\cdot\vec{x}}\right) \ . \tag{1.160b}$$

These are generalisations of the Fouriermode-expansies (1.114) and (1.115) for the linear crystal to $D = 3$ in units $\hbar = v = 1$. For calculations, it is advantageous to rewrite the preceding expressions as

$$\varphi(\vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}} \left(a(\vec{k}) + a^\dagger(-\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \tag{1.161a}$$

$$\pi(\vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} (-i) \sqrt{\frac{\omega(k)}{2}} \left(a(\vec{k}) - a^\dagger(-\vec{k})\right) e^{i\vec{k}\cdot\vec{x}} \ . \tag{1.161b}$$

As generalisation of the commutation relation (1.156) we postulate:

$$[a(\vec{k}), a(\vec{k}')] = [a^\dagger(\vec{k}), a^\dagger(\vec{k}')] = 0 \tag{1.162a}$$

$$[a(\vec{k}), a^\dagger(\vec{k}')] = \delta(\vec{k} - \vec{k}') \tag{1.162b}$$

from which the correct commutation relations (1.150) follow (at $t = 0$):

$$\begin{aligned}[\varphi(\vec{x}), \pi(\vec{y})] &= \int \frac{d^3k d^3k'}{(2\pi)^3} \frac{-i}{2} \sqrt{\frac{\omega(k')}{\omega(k)}} \left([a^\dagger(-\vec{k}), a(\vec{k}')] - [a(\vec{k}), a^\dagger(-\vec{k}')]\right) e^{i(\vec{k}\cdot\vec{x} + \vec{k}'\cdot\vec{y})} \\ &= i\delta(\vec{x} - \vec{y}) \end{aligned} \tag{1.163}$$

and where we used

$$\delta(\vec{x} - \vec{y}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} \ . \tag{1.164}$$

Analogously, we find for the Hamiltonian(1.148)

$$\begin{aligned} H &= \int d^3x \int \frac{d^3k d^3k'}{(2\pi)^3} e^{i(\vec{k}+\vec{k}')\cdot\vec{x}} \left[-\frac{\sqrt{\omega(k)\omega(k')}}{4} \left(a(\vec{k}) - a^\dagger(-\vec{k})\right) \left(a(\vec{k}') - a^\dagger(-\vec{k}')\right) \right. \\ &\quad \left. + \frac{-\vec{k}\cdot\vec{k}' + m^2}{4\sqrt{\omega(k)\omega(k')}} \left(a(\vec{k}) + a^\dagger(-\vec{k})\right) \left(a(\vec{k}') + a^\dagger(-\vec{k}')\right) \right] \\ &= \int d^3k \frac{\omega(k)}{2} \left[a^\dagger(\vec{k})a(\vec{k}) + a(\vec{k})a^\dagger(\vec{k})\right] \\ &= \int d^3k \ \omega(k) \left(a^\dagger(\vec{k})a(\vec{k}) + \frac{\delta(\vec{0})}{2}\right) \ . \end{aligned} \tag{1.165}$$

From the preceding form of the Hamiltonian, we see that a Klein–Gordon field theory is equivalent to an infinite set of harmonic oscillators labeled by the wavevector $\vec{k}$ and with angular frequency $\omega(k) = \sqrt{|\vec{k}|^2 + m^2}$. The quanta carry energy$\omega(k)$ ($\hbar = c = 1$) and are created or annihilated by $a^\dagger(\vec{k})$ en $a(\vec{k})$. Indeed, from the commutation relations (1.162) it follows that

$$[H, a^\dagger(\vec{k})] = \omega(k)a^\dagger(\vec{k}) \tag{1.166a}$$

$$[H, a(\vec{k})] = -\omega(k)a(\vec{k}) \ . \tag{1.166b}$$

The groundstate $|0\rangle$ is annihilated by all annihilators: $a(\vec{k})|0\rangle = 0, \forall \vec{k}$. All the other energy eigenstates can be obtained by applying creation operators to the groundstate:

$$|\vec{k}_1, \vec{k}_2, \cdots, \vec{k}_n\rangle = a^\dagger(\vec{k}_1)a^\dagger(\vec{k}_2)\cdots a^\dagger(\vec{k}_n)|0\rangle \ . \tag{1.167}$$

The second term in the expression (**??**) for the Hamiltonian is an infinite constant which represents the sum of the zero point energies of all oscillators. Indeed, if we restrict space to a finite cube with side L and impose periodic boundary conditions, then the wave vectors $\vec{k}$ are given by

$$\vec{k} = \frac{2\pi}{L}(n_1, n_2, n_3) \ , \qquad n_i \in \mathbb{Z} \ . \tag{1.168}$$

From this, it follows that we can replace the integrals in k-space by sums over discrete modes:

$$\int d^3k \to \frac{(2\pi)^3}{V} \sum_{\vec{k}} \tag{1.169}$$

and the Dirac-delta function can be replaced by a Kronecker-delta:

$$\delta(\vec{k} - \vec{k}') \to \left(\frac{1}{2\pi}\right)^3 \int_V d^3x e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} = \frac{V}{(2\pi)^3}\delta_{\vec{k},\vec{k}'} \tag{1.170}$$

from which

$$\delta(\vec{0}) = \frac{V}{(2\pi)^3} \ . \tag{1.171}$$

Using (1.169) and (1.171) we finaly arrive at

$$\int d^3k \frac{\omega(k)}{2}\delta(\vec{0}) \to \sum_{\vec{k}} \frac{1}{2}\omega(k) \ . \tag{1.172}$$

The groundstate has infinite energy but this infinite energy is not measurable because only energy differences are physically observable. We can therefore drop this infinite vacuum energy and this is an example of renormalisation which is ubiquitous in quantum field theory.

To prove that the quanta of the Klein–Gordon field are particles with mass m, we must show that the Einstein relation between energy and momentum is satisfied. From Noether's theorem we obtain the momentum as

$$\vec{P} = -\int d^3x \ \pi \vec{\nabla}\varphi \ . \tag{1.173}$$

By substitution of (1.161) we find using an analogous calculation as for the energy:

$$\vec{P} = \int d^3k \ \vec{k} a^\dagger(\vec{k})a(\vec{k}) \ . \tag{1.174}$$

Hence a quantum created by$a^\dagger(\vec{k})$ carries momentum $\vec{k}$. The relation between energy and momentum of a Klein–Gordon quantum is therefore

$$E(k) = \omega(k) = \sqrt{|\vec{k}|^2 + m^2} \tag{1.175}$$

which is nothing else than the Einstein relation in units $\hbar = c = 1$. From this we can conclude that the quanta of the Klein–Gordon field are particles with mass m. Because the Klein–Gordonfield is a scalar field, these particles have spin 0.

Let's consider a state of two particles with momentum$\vec{k}_1$ en $\vec{k}_2$:

$$|\vec{k}_1, \vec{k}_2\rangle = a^\dagger(\vec{k}_2) a^\dagger(\vec{k}_1)|0\rangle \tag{1.176}$$

Because of (1.162) the creation operators of Klein–Gordon particles commute and we have

$$|\vec{k}_1, \vec{k}_2\rangle = |\vec{k}_2, \vec{k}_1\rangle \ . \tag{1.177}$$

The particles of the Klein–Gordon field are therefore *bosons*.

1.7 Canonical kwantisation of the charged Klein–Gordonfield

A charged Klein–Gordonveld is a complex scalar field:

$$\phi = \frac{1}{\sqrt{2}}(\phi_1 + i\phi_2) \tag{1.178}$$

that fulfills the Klein–Gordon equation. The Lagrangian is:

$$\begin{aligned}
\mathcal{L} &= \partial_\mu \phi \partial^\mu \phi^\dagger - m^2 \phi\phi^\dagger \\
&= \frac{1}{2}\partial_\mu \phi_1 \partial^\mu \phi_1 + \frac{1}{2}\partial_\mu \phi_2 \partial^\mu \phi_2 - \frac{m^2}{2}(\phi_1^2 + \phi_2^2)
\end{aligned} \tag{1.179}$$

which is the sum of the Lagrangians of two uncharged (real) fields ϕ_1 and ϕ_2. Because ϕ, or ϕ_1 and ϕ_2,are solutions of the Klein–Gordon equation, we have the Fourier representation

$$\phi_i = \int \frac{d^3k}{\sqrt{(2\pi)^3}} \frac{1}{\sqrt{2\omega_k}} (a_i(\vec{k}) e^{-ik\cdot x} + a_i^\dagger(\vec{k}) e^{ik\cdot x}) \ , \qquad i = 1, 2 \ . \tag{1.180}$$

Let's define

$$a(\vec{k}) = \frac{1}{\sqrt{2}}[a_1(\vec{k}) + ia_2(\vec{k})] \ , \qquad a^\dagger(\vec{k}) = \frac{1}{\sqrt{2}} \ , [a_1^\dagger(\vec{k}) - ia_2^\dagger(\vec{k})] \ , \tag{1.181a}$$

$$b(\vec{k}) = \frac{1}{\sqrt{2}}[a_1(\vec{k}) - ia_2(\vec{k})] \ , \qquad b^\dagger(\vec{k}) = \frac{1}{\sqrt{2}}[a_1^\dagger(\vec{k}) + ia_2^\dagger(\vec{k})] \ . \tag{1.181b}$$

From the canonical quantisation of uncharged fields in the previous section, we find the canonical commutation relations for the a_i en $a_i^\dagger$ which we use to obtain the commutation relations for a en b:

$$[a(\vec{k}), a^\dagger(\vec{k}')] = \delta(\vec{k}-\vec{k}') \ , \qquad [b(\vec{k}), b^\dagger(\vec{k}')] = \delta(\vec{k}-\vec{k}') \ , \tag{1.182a}$$

$$[a(\vec{k}), a(\vec{k}')] = [b(\vec{k}), b(\vec{k}')] = [a(\vec{k}), b(\vec{k}')] = 0 \ , \tag{1.182b}$$

$$[a^\dagger(\vec{k}), a^\dagger(\vec{k}')] = [b^\dagger(\vec{k}), b^\dagger(\vec{k}')] = [a^\dagger(k), b^\dagger(\vec{k}')] = 0 \ . \tag{1.182c}$$

These commutation relations also follow from the canonical formalism for the ϕ-veld. Because of (1.178) and (1.180) we have the Fourier representation:

$$\phi = \int \frac{d^3k}{\sqrt{(2\pi)^3 2\omega k}} [a(\vec{k})e^{-ik\cdot x} + b^\dagger(k)e^{ik\cdot x}] \tag{1.183}$$

From(1.178) it follows that:

$$\Pi_\phi(\vec{x},t) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}(\vec{x},t)} = \dot{\phi}^\dagger(\vec{x},t) \ , \tag{1.184a}$$

$$\Pi_{\phi^\dagger}(\vec{x},t) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}^\dagger(\vec{x},t)} = \dot{\phi}(\vec{x},t) \ . \tag{1.184b}$$

The canonical commutation relations are therefore

$$[\phi(\vec{x},t), \phi(\vec{y},t)] = [\phi^\dagger(\vec{x},t), \phi^\dagger(\vec{y},t)] = 0 \ , \tag{1.185a}$$

$$[\phi(\vec{x},t), \phi^\dagger(\vec{y},t)] = 0 \tag{1.185b}$$

and

$$[\phi(\vec{x},t)], \Pi_\phi(\vec{y},t)] = [\phi(\vec{x},t), \dot{\phi}^\dagger(\vec{y},t)] = i\delta^3(\vec{x}-\vec{y}) \ , \tag{1.185c}$$

$$[\phi^\dagger(\vec{x},t), \Pi_{\phi^\dagger}(\vec{y},t)] = [\phi^\dagger(\vec{x},t), \dot{\phi}(\vec{y},t)] = i\delta^3(\vec{x}-\vec{y}) \ . \tag{1.185d}$$

From(1.185) and the Fourier representation (1.183) we also obtain the commutation relations (1.182).

Noether's theorem for U(1) transformations and charge conservation
The Lagrangian (1.178) is invariant under the global U(1)-transformations:

$$\phi \rightarrow e^{ie\chi}\phi \ , \tag{1.186a}$$

$$\phi^\dagger \rightarrow e^{-ie\chi}\phi \tag{1.186b}$$

or infinitesimally

$$\delta\phi = ie\chi\phi \ , \tag{1.187a}$$

$$\delta\phi^\dagger = -ie\chi\phi^\dagger \ . \tag{1.187b}$$

This means that the variation of the Lagrangian vanishes is under (1.187) or

$$\begin{aligned} \delta\mathcal{L} = 0 &= \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial\partial^\mu\phi}\delta\partial^\mu\phi \\ &+ \frac{\partial\mathcal{L}}{\partial\phi^\dagger}\delta\phi^\dagger + \frac{\partial\mathcal{L}}{\partial\partial^\mu\phi^\dagger}\delta\partial^\mu\phi^\dagger \ . \end{aligned} \tag{1.188}$$

From

$$\delta\partial^\mu\phi = ie\chi\partial^\mu\phi \tag{1.189a}$$

$$\delta\partial^\mu\phi^\dagger = -ie\chi\partial^\mu\phi^\dagger \tag{1.189b}$$

and the Euler-Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial\phi} - \partial^\mu\frac{\partial\mathcal{L}}{\partial\partial^\mu\phi} = 0 \tag{1.190a}$$

$$\frac{\partial\mathcal{L}}{\partial\phi^\dagger} - \partial^\mu\frac{\partial\mathcal{L}}{\partial\partial^\mu\phi^\dagger} = 0 \tag{1.190b}$$

it follows that

$$ie\chi\left[\partial^\mu\frac{\partial\mathcal{L}}{\partial\partial^\mu\phi}\phi + \frac{\partial\mathcal{L}}{\partial\partial^\mu\phi}\partial^\mu\phi - \partial^\mu\frac{\partial\mathcal{L}}{\partial\partial^\mu\phi^\dagger}\phi^\dagger - \frac{\partial\mathcal{L}}{\partial\partial^\mu\phi^\dagger}\partial^\mu\phi^\dagger\right] = 0 \ , \tag{1.191}$$

or after deviding by $-\chi$:

$$\partial^\mu j_\mu = 0 \tag{1.192}$$

with

$$j_\mu = ie\left[\frac{\partial\mathcal{L}}{\partial\partial^\mu\phi^\dagger}\phi^\dagger - \frac{\partial\mathcal{L}}{\partial\partial^\mu\phi}\phi\right] \ . \tag{1.193}$$

Using the charged Klein–Gordon Lagrangian, we finally obtain

$$j_\mu = ie[\partial_\mu\phi\phi^\dagger - \partial_\mu\phi^\dagger\phi] \ . \tag{1.194}$$

From Noether's theorem we find a conserved current for the global U(1)-symmetry given by (1.194). The corresponding charge is

$$Q = \int d^3x \ j_0 = ie\int d^3x[\dot{\phi}\phi^\dagger - \dot{\phi}^\dagger\phi] \ . \tag{1.195}$$

After substition of the Fourierr epresentation (1.183) we find for the charge:

$$Q = e\int d^3k[a^\dagger(\vec{k})a(\vec{k}) - b^\dagger(\vec{k})b(\vec{k})] \ . \tag{1.196}$$

Therefore, the $a^\dagger(\vec{k})$ create particles with charge e and the $b^\dagger(\vec{k})$ antiparticles with charge $-e$.

1.8 Non-relativistic quantum field theory.

Assume we have a classical scalar field $\psi(\vec{x},t)$ which obeys the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(\vec{x})\psi \tag{1.197}$$

and which we want to quantize. The wavefunction ψ can be viewed as a classical field. If we quantize this classical field, this is sometimes called "second quantization". The classical equation (1.197) describes the quantum behaviour of one particle. We will show that quantizing the Schrödinger field ψ turns the one particle quantum theory into a many body theory.

To quantize the Schrödinger field we will as usual go over to the Hamiltonian formalism. It is easy to check that the Schrödinger equation can be derived from the Lagrangian density

$$\mathcal{L} = i\hbar\psi^*\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2m}\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi - V(\vec{x})\psi^*\psi\ . \tag{1.198}$$

Indeed, variation with respect to ψ^* yields

$$\begin{aligned}\partial_\mu\frac{\partial\mathcal{L}}{\partial_\mu\psi^*} - \frac{\partial\mathcal{L}}{\partial\psi^*} &= \partial_t\frac{\partial\mathcal{L}}{\partial\dot{\psi}^*} - \vec{\nabla}\cdot\frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\psi^*)} - \frac{\partial\mathcal{L}}{\partial\psi^*}\\ &= i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\psi - V(\vec{x})\psi = 0\ .\end{aligned} \tag{1.199}$$

The canonically conjugate momentum forψ is

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\psi}} = i\hbar\psi^*\ . \tag{1.200}$$

The Hamiltonian density then becomes

$$\mathcal{H} = \pi\dot{\psi} - \mathcal{L} = \frac{\hbar^2}{2m}\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi + V(\vec{x})\psi^*\psi\ , \tag{1.201}$$

so that we find after partial integration:

$$H = \int d^3x\ \mathcal{H} = \int d^3x\ \psi^*(\vec{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x})\ . \tag{1.202}$$

We can quantize by imposing the canonical commutation relations:

$$[\hat{\psi}(\vec{x},t),\hat{\pi}(\vec{y},t)] = i\hbar\delta(\vec{x}-\vec{y}) \tag{1.203a}$$

$$[\hat{\psi}(\vec{x},t),\hat{\psi}(\vec{y},t)] = [\hat{\pi}(\vec{x},t),\hat{\pi}(\vec{y},t)] = 0\ . \tag{1.203b}$$

Because of (1.200) these become

$$[\hat{\psi}(\vec{x},t),\hat{\psi}^\dagger(\vec{y},t)] = \delta(\vec{x}-\vec{y}) \tag{1.204a}$$

$$[\hat{\psi}(\vec{x},t),\hat{\psi}(\vec{y},t)] = [\hat{\psi}^\dagger(\vec{x},t),\hat{\psi}^\dagger(\vec{y},t)] = 0\ . \tag{1.204b}$$

We now develop the wave operators $\hat{\psi}$ en $\hat{\psi}^\dagger$ in normal modes which are solutions of the time independent Schrödinger equation:

$$\hat{\psi}(\vec{x},t) = \sum_i \hat{a}_i(t) u_i(\vec{x}) \tag{1.205}$$

with

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right] u_i(\vec{x}) = \epsilon_i u_i(\vec{x}) \ . \tag{1.206}$$

From the orthonormality conditions and the completness relation

$$\int d^3x \ u_i^*(\vec{x}) u_j(\vec{x}) = \delta_{ij} \tag{1.207a}$$

$$\sum_i u_i(\vec{x}) u_i^*(\vec{x}') = \delta(\vec{x}-\vec{x}') \tag{1.207b}$$

it easily follows that the commutation relations are obeyed if

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \tag{1.208a}$$

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \ . \tag{1.208b}$$

Substituting the normal mode expansion (1.205) into the Hamiltonian (1.202), we finally obtain:

$$\hat{H} = \sum_i \hat{a}_i^\dagger \hat{a}_i \epsilon_i \tag{1.209}$$

or

$$\hat{H} = \sum_i \hat{n}_i \epsilon_i \tag{1.210}$$

with $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$, the number operator which counts the number of particles in the i-the eigenstate.

The interpretation of the previous paragraph is straightforward. Second quantization allows us to describe non-relativistic many body systems with a variable number of particles. These particles are moving in an external potential $V(\vec{x})$ and the number of particles that are in the i-th energy eigenstate of the one particle Hamiltonian is counted by $\hat{n}_i$.The formula (1.210) for the Hamiltonian $\hat{H}$ is then self explanatory.

Let's take as a special case $V(\vec{x}) = 0$, then we have a continuous spectrum

$$\epsilon(\vec{k}) = \frac{\hbar^2}{2m} k^2 \tag{1.211}$$

with eigenmodes

$$u(\vec{k},\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}} \ . \tag{1.212}$$

The mode expansion then becomes

$$\hat{\psi}(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} \hat{a}(\vec{k},t) e^{i\vec{k}\cdot\vec{x}} \ . \tag{1.213}$$

The operator $\hat{a}(\vec{k},t)$ annihilates a non-relativistic particle with momentum $\vec{p} = \hbar\vec{k}$. Because we can go over with a Fourier transform from momentum space to configuration space (position space), it follows from (1.213) that $\hat{\psi}(\vec{x},t)$ annihilates a particle on postion $\vec{x}$, while $\hat{\psi}^\dagger(\vec{x},t)$ creates a particle on position $\vec{x}$. Non-relativistic quantum field operators are hence annihilation or creation operators in configuration space.

Because of the commutation relations (1.204) , the particles described by $\hat{\psi}$ and $\hat{\psi}^\dagger$are bosons. If we want to describe non-relativistic fermions, it suffices to impose anticommutation relations:

$$\{\hat{a}_i, \hat{a}_j\}_+ = \{\hat{a}_i^\dagger, \hat{a}_i^\dagger\}_+ = 0 \tag{1.214a}$$

$$\{\hat{a}_i, \hat{a}_j^\dagger\}_+ = \delta_{ij} \tag{1.214b}$$

with $\{\hat{A}, \hat{B}\}_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$. Indeed let

$$|i_1, i_2\rangle = \hat{a}_{i_1}^\dagger \hat{a}_{i_2}^\dagger |\Theta\rangle \tag{1.215}$$

with $\hat{a}_i|\Theta\rangle = 0$, $\forall i$, then from$\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$ it follows that

$$\begin{aligned} |i_1, i_2\rangle &= \hat{a}_{i_1}^\dagger \hat{a}_{i_2}^\dagger |\Theta\rangle \\ &= -\hat{a}_{i_2}^\dagger \hat{a}_{i_1}^\dagger |\Theta\rangle = -|i_2, i_1\rangle \ . \end{aligned} \tag{1.216}$$

Consequently these particles behave as fermions. Also the interpretation of $\hat{a}_i$ and $\hat{a}_i^\dagger$ as annihilation and creation operators remains valid. Indeed:

$$\begin{aligned} [\hat{H}, \hat{a}_i] &= \left[\sum_j \hat{a}_j^\dagger \hat{a}_j \epsilon_j, \hat{a}_i\right] \\ &= \sum_j \epsilon_j (\hat{a}_j^\dagger \hat{a}_j \hat{a}_i - \hat{a}_i \hat{a}_j^\dagger \hat{a}_j) \\ &= \sum_j \epsilon_j (\hat{a}_j^\dagger \{\hat{a}_j, \hat{a}_i\}_+ - \hat{a}_j^\dagger \hat{a}_i \hat{a}_j - \{\hat{a}_i, \hat{a}_j^\dagger\}_+ \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \hat{a}_j) \\ &= -\epsilon_i \hat{a}_i \ , \end{aligned} \tag{1.217}$$

so that $\hat{a}_i$ annihilates a particle in the i-th mode . Furthermore, from

$$\{\hat{a}_i^\dagger, \hat{a}_i^\dagger\}_+ = 0 = 2(\hat{a}_i^\dagger)^2 \tag{1.218}$$

we recover that not more then one particle can be in the i-th mode.

If we substitute the anticommutation relations of $\hat{a}_i$ en $\hat{a}_i^\dagger$ in the mode expansions, we finally obtain the canonical anticommutation relations for the fermionic field operators:

$$\{\hat{\psi}(\vec{x},t), \hat{\psi}(\vec{y},t)\}_+ = \{\hat{\psi}^\dagger(\vec{x},t), \hat{\psi}^\dagger(\vec{y},t)\}_+ = 0 \tag{1.219a}$$

$$\{\hat{\psi}(\vec{x},t), \hat{\psi}^\dagger(\vec{y},t)\}_+ = \delta(\vec{x} - \vec{y}) \ . \tag{1.219b}$$

1.9 Canonical quantization of the Dirac field.

Electrons have spin 1/2 and obey Fermi statistics; consequently, for the quantization of relativistic electrons described by the Dirac equation, we will have to impose canonical anticommutation relations on the canonically conjugate fields.

The Dirac equation for a relativistic particle with spin 1/2 is:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar c}{i}\left(\alpha_1\frac{\partial}{\partial x^1} + \alpha_2\frac{\partial}{\partial x^2} + \alpha_3\frac{\partial}{\partial x^3}\right)\psi + \beta mc^2\psi \tag{1.220}$$

with ψ a wavefunction with four components ψ_α (*Dirac spinor*) and α_i and β hermitian 4×4-matrices which obey anticommutation relations:

$$\{\alpha_i,\alpha_j\} = 2\delta_{ij}\mathbb{1} \tag{1.221a}$$
$$\{\alpha_i,\beta\} = 0 \tag{1.221b}$$
$$\alpha_i^2 = \beta^2 = \mathbb{1}\ . \tag{1.221c}$$

In the Dirac representation we have:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\ , \qquad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\ . \tag{1.222}$$

Introducing the relativistic notation

$$\gamma^i = \beta\alpha_i\ , \qquad \gamma^0 = \beta \tag{1.223}$$

and choosing natural units $\hbar = c = 1$, the Dirac equation becomes after multiplication with β:

$$i\gamma^\mu\partial_\mu\psi - m\psi = 0\ . \tag{1.224}$$

The matrices γ^μ are the so called Dirac matrices and because of (2.140) and (2.142) they obey the anticommutation relations:

$$\{\gamma^\mu,\gamma^\nu\} = 2g^{\mu\nu}\mathbb{1}\ . \tag{1.225}$$

In the Dirac representation th γ-matrices are given by:

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\ , \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}\ . \tag{1.226}$$

Introducing the notation $\not{a} = \gamma^\mu a_\mu$, we obtain a compact form of the Dirac equation:

$$(i\not{\partial} - m)\psi = 0\ . \tag{1.227}$$

Under a Lorentz transformation

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{1.228}$$

the Dirac wavefunction transforms as

$$\psi(x) \to \psi'(x') = \mathcal{D}(\Lambda)\psi(x) \ . \tag{1.229}$$

The Dirac equation (1.224) is invariant under the Lorentz transformation (1.228), (1.229) if

$$\mathcal{D}(\Lambda)\gamma^\mu \mathcal{D}(\Lambda)^{-1}\Lambda^\nu{}_\mu = \gamma^\nu \ . \tag{1.230}$$

From this it follows that

$$\mathcal{D}(\Lambda) = \exp -\frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu} \tag{1.231}$$

with

$$\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu] \tag{1.232}$$

the generators of the Lorentz group.

Because $(\gamma^0)^2 = \mathbb{1}$ and the Dirac matrices anticommute for $\mu \neq \nu$, we have

$$\gamma^0 = \gamma^0\gamma^0\gamma^0 \tag{1.233a}$$
$$-\gamma^i = \gamma^0\gamma^i\gamma^0 \ . \tag{1.233b}$$

On the other hand, from the Hermiticity of α_i en β it follows that

$$(\gamma^0)^\dagger = \beta^\dagger = \beta = \gamma^0 \tag{1.234a}$$
$$(\gamma^i)^\dagger = (\beta\alpha_i)^\dagger = \alpha_i\beta = -\beta\alpha_i = -\gamma^i \ , \tag{1.234b}$$

so that

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0 \ . \tag{1.235}$$

From (1.232) we immediately get that $\sigma^\dagger_{\mu\nu} = -\gamma_0\sigma_{\mu\nu}\gamma_0$, and hence:

$$\mathcal{D}(\Lambda)^\dagger = \gamma^0\mathcal{D}(\Lambda)^{-1}\gamma^0 \ . \tag{1.236}$$

If we define the conjugate spinor $\overline{\psi}$ as

$$\overline{\psi} = \psi^\dagger\gamma^0 \ , \tag{1.237}$$

then it follows from (1.230) and (1.236) that

$$J^\mu = \overline{\psi}\gamma^\mu\psi \tag{1.238a}$$
$$S = \overline{\psi}\psi \tag{1.238b}$$

respectively form a Lorentz fourvector and a Lorentz scalar vormen. Furhtermore, from the Dirac equation, it follows that

$$\partial_\mu(\overline{\psi}\gamma^\mu\psi) = 0 \ , \tag{1.239}$$

so that $\overline{\psi}\gamma^\mu\psi$ is the conserved probability current and $\overline{\psi}\gamma^0\psi = \psi^\dagger\psi$ the probability density.

One can easily check that the Dirac equation (1.224) is invariant under parity transformations $\vec{x} \to -\vec{x}, t \to t$, if

$$\psi \to P\psi = \gamma^0 \psi \ . \tag{1.240}$$

The matrix γ_5 defined by

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 \tag{1.241}$$

anticommutes with all Diracmatrices γ_μ:

$$\{\gamma_\mu, \gamma_5\} = 0 \ . \tag{1.242}$$

From this we find that $\{\gamma_5, P\} = [\gamma_5, \mathcal{D}(\Lambda)] = 0$ so that

$$A_\mu = \overline{\psi}\gamma_\mu\gamma_5\psi \tag{1.243a}$$
$$P = \overline{\psi}\gamma_5\psi \tag{1.243b}$$

are respectively an axial Lorentz fourvector and a pseudoscalar. We can now form a Lorentz invariant which is a function of ψ and $\psi^\dagger$ and which after variation with respect to $\overline{\psi}$ gives the Dirac equation (1.227) :

$$\mathcal{L} = \overline{\psi}(i\partial\!\!\!/ - m)\psi \ . \tag{1.244}$$

The Dirac equation has plane wave solutions with positive and negative energy:

$$\psi^{(+),s} = e^{-ip\cdot x}u^s(p) = e^{-iE(p)t}e^{i\vec{p}\cdot\vec{x}}u^s(p) \tag{1.245a}$$
$$\psi^{(-),s} = e^{ip\cdot x}v^s(p) = e^{iE(p)t}e^{-i\vec{p}\cdot\vec{x}}v^s(p) \tag{1.245b}$$

with $s = \pm 1$ the helicity and $E(p) = \sqrt{|\vec{p}|^2 + m^2}$. After substitution in the Dirac equation (1.227) we obtain the equation for the plane wave spinors

$$(p\!\!\!/ - m)u^s(p) = 0 \tag{1.246a}$$
$$(p\!\!\!/ + m)v^s(p) = 0 \ . \tag{1.246b}$$

In the rest frame where $p^\mu = (m, \vec{0})$, we have$p\!\!\!/ = E\gamma^0 = m\gamma^0$, so that (1.246) simplifies to

$$\gamma^0 u = u \tag{1.247a}$$
$$\gamma^0 v = -v \ . \tag{1.247b}$$

In the Dirac representation, (1.247) has the general solutions

$$u = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} \ , \qquad v = \begin{pmatrix} 0 \\ \chi \end{pmatrix} \tag{1.248}$$

with φ and χ arbitrary two-component spinors. In the Dirac representation, in the rest frame, the first two components of a Dirac spinor describe the positive energy part and the last two the negative energy part. As basis for φ and χ we can choose the helicity eigenspinors φ^s, $s = \pm 1$, which obey

$$\frac{\vec{\sigma}\cdot\vec{p}}{|\vec{p}|}\varphi^s = s\varphi^s \ . \tag{1.249}$$

Using the identity

$$(\not{p} - m)(\not{p} + m) = p^2 - m^2 = 0 \tag{1.250}$$

the plane wave spinors u en v are given in an arbitrary frame by

$$\begin{aligned} u^s(p) &= \frac{\not{p} + m}{\sqrt{2m(E+m)}} u^s && (1.251a) \\ v^s(p) &= \frac{-\not{p} + m}{\sqrt{2m(E+m)}} v^s && (1.251b) \end{aligned}$$

with

$$u^s = \begin{pmatrix} \varphi^s \\ 0 \end{pmatrix} , \qquad v^s = \begin{pmatrix} 0 \\ \varphi^{-s} \end{pmatrix} . \tag{1.252}$$

Because u^s and v^s fulfill $\overline{u}^s u^{s'} = \delta_{ss'}$, $\overline{v}^s v^{s'} = -\delta_{ss'}$, $\overline{u}v = 0$, and because $\overline{\psi}\psi$ is a Lorentz scalar, $u^s(p)$ and $v^s(p)$ are normalised as

$$\begin{aligned} \overline{u}^s(p) u^{s'}(p) &= \delta_{ss'} , \qquad \overline{u}^s(p) v^{s'}(p) = 0 && (1.253a) \\ \overline{v}^s(p) v^{s'}(p) &= -\delta_{ss'} , \qquad \overline{v}^s(p) u^{s'}(p) = 0 && (1.253b) \end{aligned}$$

or

$$\begin{aligned} u_s^\dagger(p) u_s(p) &= \frac{E(p)}{m} \delta_{ss'} && (1.254a) \\ v_s^\dagger(p) v_s(p) &= \frac{E(p)}{m} \delta_{ss'} . && (1.254b) \end{aligned}$$

The probability densities transform as the fourth component of a Lorentz fourvector, as was to be expected.

In the rest frame, the projectors on postive and negative energy are given by

$$\begin{aligned} \Lambda_+ &= \frac{1 + \gamma_0}{2} = \frac{p^0\gamma^0 + m}{2m} = \frac{\not{p} + m}{2m} && (1.255a) \\ \Lambda_- &= \frac{1 - \gamma_0}{2} = \frac{-p^0\gamma^0 + m}{2m} = \frac{-\not{p} + m}{2m} . && (1.255b) \end{aligned}$$

In an arbitrary frame we obtain because of (1.253) the following Lorentz invariant expressions for these projectors:

$$\begin{aligned} \Lambda_+(p) &= \sum_s u^s(p) \overline{u}^s(p) = \frac{\not{p} + m}{2m} && (1.256a) \\ \Lambda_-(p) &= -\sum_s v^s(p) \overline{v}^s(p) = \frac{-\not{p} + m}{2m} . && (1.256b) \end{aligned}$$

The Lorentz invariant Lagrangian (1.244) for the Dirac field can be rewritten as

$$\mathcal{L} = \overline{\psi}(i\gamma^\mu \partial_\mu - m)\psi = i\psi^\dagger \dot{\psi} + i\psi^\dagger \vec{\alpha} \cdot \vec{\nabla}\psi - m\psi^\dagger \beta \psi \tag{1.257}$$

where we used $\beta = \gamma^0$, $\beta^2 = 1$, $\vec{\alpha} = \gamma^0\vec{\gamma}$ en $\overline{\psi} = \psi^\dagger\psi^0$. Because ψ and $\psi^\dagger$ are independent fields, we have

$$\frac{\partial \mathcal{L}}{\partial \dot{\psi}_\alpha} = i\psi_\alpha^\dagger \ , \qquad \frac{\partial \mathcal{L}}{\partial \dot{\psi}_\alpha^\dagger} = 0 \ , \tag{1.258}$$

and hence:

$$\pi_{\psi_\alpha} = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_\alpha} = i\psi_\alpha^\dagger \ , \qquad \pi_{\psi_\alpha^\dagger} = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_\alpha^\dagger} = 0 \ . \tag{1.259}$$

The Hamiltonian density is defined in the usual way:

$$\begin{aligned} \mathcal{H} &= \pi_{\psi_\alpha}\dot{\psi}_\alpha + \pi_{\psi_\alpha^\dagger}\dot{\psi}_\alpha^\dagger - \mathcal{L} \\ &= i\psi^\dagger\dot{\psi} - (i\psi^\dagger\dot{\psi} + i\psi^\dagger\vec{\alpha}\cdot\vec{\nabla}\psi - m\psi^\dagger\beta\psi) \\ &= \psi^\dagger(-i\vec{\alpha}\cdot\vec{\nabla} + \beta m)\psi \ . \end{aligned} \tag{1.260}$$

The field Hamiltonian is thus given by the expectation value of the one particle Dirac Hamiltonian$H_\mathrm{D} = \vec{\alpha}\cdot\vec{p} + \beta m$:

$$H = \int d^3x \ \psi^\dagger(-i\vec{\alpha}\cdot\vec{\nabla} + \beta m)\psi \ . \tag{1.261}$$

The canonical anticommutation relations are now because of $\pi_\psi = i\psi^\dagger$:

$$\{\psi_\alpha(\vec{x},t), \psi_\beta(\vec{y},t)\}_+ = \{\psi_\alpha^\dagger(\vec{x},t), \psi_\beta^\dagger(\vec{y},t)\}_+ \tag{1.262a}$$

$$\{\psi_\alpha(\vec{x},t), \psi_\beta^\dagger(\vec{y},t)\}_+ = \delta_{\alpha\beta}\delta^3(\vec{x}-\vec{y}) \ . \tag{1.262b}$$

In analogy to the complex Klein–Gordon field, we propose the following mode expansion in plane waves :

$$\psi(\vec{x},t) = \sum_s \int \frac{d^3p}{(2\pi)^{3/2}}\sqrt{\frac{m}{E(p)}}\left(a(\vec{p},s)u^s(\vec{p})e^{i\vec{p}\cdot\vec{x}-iE(p)t} + b^\dagger(\vec{p},s)v^s(\vec{p})e^{i\vec{p}\cdot\vec{x}+iE(p)t}\right) \ . \tag{1.263}$$

Here $a(\vec{p},s)$ is an annihilation operator for the Dirac particles with momentum $\vec{p}$ and helicity s while $b^\dagger(\vec{p},s)$ creates a Dirac-antiparticle with momentum $\vec{p}$ and helicity s. The latter can be seen from the fact that $v(\vec{p},s)$ is a plane wave spinor with momentum $-\vec{p}$, helicity $-s$ and energy $-E(p)$ and we can interpret $b^\dagger(\vec{p},s) = d(-\vec{p},-s)$ as an annihilator of a particle with negative energy, momentum and helicity $-\vec{p}$ and $-s$, and hence as the creator of a particle with positive energy and momentum and helicity $\vec{p}$ and s. By using (1.254) one can easily show that the anticommutation relations in configuration space , when transformed to momentum space become

$$\{a(p,s), a(p',s')\} = \{b(p,s), b(p',s')\} = 0 \tag{1.264a}$$

$$\{a^\dagger(p,s), a^\dagger(p',s')\} = \{b^\dagger(p,s), b^\dagger(p',s')\} = 0 \tag{1.264b}$$

$$\{a(p,s), a^\dagger(p',s')\} = \{b(p,s), b^\dagger(p',s')\} = \delta_{s,s'}\delta(\vec{p}-\vec{p}') \tag{1.264c}$$

$$\{a,b\} = \{a,b^\dagger\} = \{a^\dagger,b\} = \{a^\dagger,b^\dagger\} = 0 \ . \tag{1.264d}$$

The Hamiltonian (1.261) becomes after substitution of the mode expansion (1.263):

$$\begin{aligned} H &= \sum_s \int d^3p\ E(p) \left[a^\dagger(\vec{p},s)a(p,s) - b(\vec{p},s)b^\dagger(\vec{p},s)\right] \\ &= \sum_s \int d^3p\ E(p) \left[a^\dagger(\vec{p},s)a(\vec{p},s) + b^\dagger(\vec{p},s)b(\vec{p},s)\right] \\ &\quad -\sum_s \int d^3p\ E(p)\delta(\vec{0})\ . \end{aligned} \tag{1.265}$$

Analogously, we find for the momentum operator $\vec{P}$, which is the "expectation value" for the field ψ of the momentum operator $\hat{\vec{P}} = -i\vec{\nabla}$:

$$\vec{P} = \int d^3x\ \psi^\dagger(-i\vec{\nabla})\psi = \sum_s \int d^3p\ \vec{p}[a^\dagger(\vec{p},s)a(\vec{p},s) + b^\dagger(\vec{p},s)b(\vec{p},s)]\ . \tag{1.266}$$

The quanta of the Dirac field therefore obey the Einstein relation between energy and momentum and hence are relativistic particles. Because of the spinor character of ψ , they have spin 1/2 and because of the anticommutation relations, they are fermions:

$$a^\dagger(\vec{p}_1,s_1)a^\dagger(\vec{p}_2,s_2)|\Theta\rangle = |\vec{p}_1,s_1;\vec{p}_2,s_2\rangle \tag{1.267}$$

and

$$|\vec{p}_1,s_1;\vec{p}_2,s_2\rangle = -|\vec{p}_2,s_2;\vec{p}_1,s_1\rangle\ . \tag{1.268}$$

Just as the charged Klein–Gordon field, the Dirac field has a global U(1)-symmetrie:

$$\psi \rightarrow e^{ie\chi}\psi \tag{1.269a}$$

$$\psi^\dagger \rightarrow e^{-ie\chi}\psi^\dagger \tag{1.269b}$$

with conserved Noether current (exercise):

$$j_\mu = e\overline{\psi}\gamma_\mu\psi \tag{1.270}$$

which is the electric current density fourvector. The corresponding conserved charge is the electric charge

$$\begin{aligned} Q &= e\int d^3x\ \psi^\dagger\psi \\ &= e\sum_s \int d^3p[a^\dagger(\vec{p},s)a(\vec{p},s) + b(\vec{p},s)b^\dagger(\vec{p},s)] \\ &= e\sum_s \int d^3p[a^\dagger(\vec{p},s)a(\vec{p},s) - b^\dagger(\vec{p},s)b(\vec{p},s)] + e\sum_s \int d^3p\ \delta(0)\ . \end{aligned} \tag{1.271}$$

From this, it follows that the Dirac antiparticle created by $b^\dagger$ has opposite charge. The best known Dirac particle is the electron with as antiparticle the positron .

1.10 Canonical quantisation of the Maxwell field.

The Maxwell equations with source term are:

$$\vec{\nabla}\cdot\vec{E} = \rho \; , \qquad \vec{\nabla}\cdot\vec{B} = 0 \; , \tag{1.272a}$$

$$\vec{\nabla}\times\vec{B} = \frac{\partial}{\partial t}\vec{E} + \vec{j} \; , \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial}{\partial t}\vec{B} \tag{1.272b}$$

. If we introduce the fourvector potential A^μ with

$$\vec{E} = -\vec{\nabla}A_0 - \frac{\partial}{\partial t}\vec{A} \; , \qquad \vec{B} = \vec{\nabla}\times\vec{A} \tag{1.273}$$

they can be rewritten in a manifestly Lorentz covariant way as

$$\partial_\mu F^{\mu\nu} = j^\nu \tag{1.274}$$

with

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu \tag{1.275}$$

the electromagnetic tensor. Because $F^{\mu\nu}$ is antisymmetric we have

$$\partial_\nu\partial_\mu F^{\mu\nu} = \partial_\nu j^\nu = 0 \tag{1.276}$$

so that the current j^ν is conserved. The Maxwell equations can be obtained by variation of the Lagrangian

$$\mathcal{L} = \mathcal{L}_{\text{Max}} + \mathcal{L}_{\text{int}} \tag{1.277}$$

where the free Maxwell Lagrangian is given by

$$\mathcal{L}_{\text{Max}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} \tag{1.278}$$

and the interaction Lagrangian by

$$\mathcal{L}_{\text{int}} = -j_\mu A^\mu \; . \tag{1.279}$$

Because $F^{\mu\nu}$ is invariant under the gauge transformation

$$A^\mu \to A^\mu + \partial^\mu \chi \tag{1.280}$$

or

$$\begin{aligned} A^0 &\to A^0 + \frac{\partial}{\partial t}\chi \\ \vec{A} &\to \vec{A} - \vec{\nabla}\chi \end{aligned} \tag{1.281}$$

the Maxwell equations themselves are invariant under these gauge transformations. This means that the time evolution of the fields A^μ is not fully determined by the equations of motion and there will be difficulties when trying to apply the canonical quantisation formalism.

Indeed: let's calculate the canonically conjugate fields of $A^\mu = (A_0, \vec{A})$:

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial \partial_0 A_\mu} = F^{\mu 0} \tag{1.282}$$

or

$$\pi^0 = 0 \ , \qquad \pi^i = E^i \ . \tag{1.283}$$

The canonically conjugate field of the vector potential $\vec{A}$ is the electric field $\vec{E}$, but the canonically conjugate field of the potential A^0 is identically zero. So we cannot quantize the A^0 field by simply imposing canonical commutation relations because ($[A_0(\vec{x}), \pi_0(\vec{y})] = 0$).

Fermi found an elegant solution to this problem by using the gauge invariance in a clever way. The Maxwell equations (1.272) determine A^μonly up to gauge transformations $A^\mu \to A^\mu + \partial^\mu \chi$. We still have the freedom to choose a gauge condition such as the Lorentz gauge

$$\partial_\mu A^\mu = 0 \ . \tag{1.284}$$

It is always possible to bring the field A^μ in this gauge. Indeed , the gauge transformed field $A^{\mu\prime}$

$$A^{\mu\prime} = A^\mu - \partial^\mu \left(\frac{1}{\Box} \partial_\nu A^\nu \right) \tag{1.285}$$

fulfills the Lorentz gauge. We can now choose a new Lagrangian for the Maxwell field that is equivalent to the original one in the Lorentz gauge:

$$\mathcal{L}'_{\text{Max}} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} \lambda (\partial_\nu A^\nu)^2 \tag{1.286}$$

where λ is a gauge parameter that can be freely chosen. The extra term in $\mathcal{L}'$ is called the *gauge fixing term*. The Euler-Lagrange equations are now:

$$\partial_\mu F^{\mu\nu} + \lambda \partial^\nu (\partial_\mu A^\mu) = 0 \ . \tag{1.287}$$

If we take the covariant divergence of these field equations, we obtain

$$\partial_\mu \partial_\nu F^{\mu\nu} + \lambda \partial_\nu \partial^\nu (\partial_\mu A^\mu) = 0 \ . \tag{1.288}$$

Because of the antisymmetry of $F^{\mu\nu}$ we have $\partial_\mu \partial_\nu F^{\mu\nu} = 0$, so that

$$\Box (\partial_\mu A^\mu) = 0 \ . \tag{1.289}$$

Therefore the field $\partial_\mu A^\mu$ is a free field. Imposing the initial conditions at $t = 0$:

$$\partial_\mu A^\mu(\vec{x}, 0) = 0 \tag{1.290a}$$
$$\partial_0 \partial_\mu A^\mu(\vec{x}, 0) = 0 \tag{1.290b}$$

, it follows from (1.289) that

$$\partial_\mu A^\mu(\vec{x}, t) = 0 \qquad \forall t \ , \tag{1.291}$$

so that the modified Euler-Lagrange equations (1.287) reduce to the usual free Maxwell equations

$$\partial_\mu F^{\mu\nu} = 0 \ . \tag{1.292}$$

Thus, we have found a new Lagrangian which, if we impose appropriate initial conditions, generates the same solutions as the ones of the Maxwell equations in the Lorentz gauge. For the special choice $\lambda = 1$, the Euler Lagrange equations (1.287) reduce to

$$\begin{aligned} 0 &= \partial_\mu F^{\mu\nu} + \partial^\nu(\partial_\mu A^\mu) \\ &= \partial_\mu(\partial^\mu A^\nu - \partial^\nu A^\mu) + \partial^\nu \partial_\mu A^\mu \\ &= \Box A^\nu \ , \end{aligned} \tag{1.293}$$

so that the Maxwell field A^μ obeys the massless Klein–Gordon equations. These equations are precisely the Maxwell equations in the Lorentz gauge. In this case we can rewrite the Lagrangian as:

$$\begin{aligned} \mathcal{L}'_{\text{Max}} &= -\frac{1}{2}(\partial_\mu A_\nu - \partial_\nu A_\mu)\partial^\mu A^\nu - \frac{1}{2}\partial_\mu A^\mu \partial_\nu A^\nu \\ &= -\frac{1}{2}\partial_\mu A_\nu \partial^\mu A^\nu + \frac{1}{2}\partial_\nu(A_\mu \partial^\mu A^\nu - A^\nu \partial_\mu A^\mu) \ , \end{aligned} \tag{1.294}$$

so that by dropping the last term which is a total divergence we finally obtain:

$$\begin{aligned} \mathcal{L}''_{\text{Max}} &= -\frac{1}{2}\partial_\mu A_\nu \partial^\mu A^\nu \\ &= -\frac{1}{2}\partial_\mu A_0 \partial^\mu A_0 + \frac{1}{2}\partial_\mu A_i \partial^\mu A_i \ . \end{aligned} \tag{1.295}$$

The Lagrangian for the spacial components A_i is the massless Klein–Gordon-Lagrangian; for the time component A_0 however there is an extra minus sign. But they all obey the massless Klein–Gordon equation.

The canonically conjugate momentum of the Maxwell field A_μ is now:

$$\pi^\mu = \frac{\partial \mathcal{L}''_{\text{Max}}}{\partial \partial_0 A^\mu} = -\partial^0 A^\mu \ . \tag{1.296}$$

so that space and time components now behave in the same way. The Hamiltonian density is

$$\begin{aligned} \mathcal{H} &= \pi^\mu \dot{A}_\mu - \mathcal{L}''_{\text{Max}} \\ &= \partial^0 A^\mu \partial^0 A_\mu - \frac{1}{2}\partial^0 A^\mu \partial^0 A_\mu + \frac{1}{2}\vec{\nabla} A^\mu \cdot \vec{\nabla} A_\mu \\ &= \frac{1}{2}\dot{A}^\mu \dot{A}_\mu + \frac{1}{2}\vec{\nabla} A^\mu \cdot \vec{\nabla} A_\mu \\ &= \frac{1}{2}\sum_{i=1}^{3}(\dot{A}_i^2 + (\vec{\nabla} A_i)^2) - \frac{1}{2}(\dot{A}_0^2 + (\vec{\nabla} A_0)^2) \ . \end{aligned} \tag{1.297}$$

The Hamiltonian density looks like the one of four uncharged massless Klein–Gordon fields with this important difference that the part for A^0 has a negative sign. At first view, this Hamiltonian does not look positive definite and we expect some difficulties for the physical interpretation. Furthermore we have four polarisations (three spacial ones and one temporal) while we know that an electromagnetic wave has only two independent polarisations. All these problems can now be solved by a quantum implementation of the Lorentz gauge.

Canonical quantisation procedes in the usual way by imposing the canonical commutation relations

$$[A^\mu(\vec{x},t), A^\nu(\vec{y},t)] = [\pi^\mu(\vec{x},t), \pi^\nu(\vec{y},t)] = 0 \tag{1.298a}$$

$$[A^\mu(\vec{x},t), \pi^\nu(\vec{y},t)] = ig^{\mu\nu}\delta(\vec{x}-\vec{y}) \ . \tag{1.298b}$$

Because $\pi^\mu = -\partial^0 A^\mu$ this last commutation relation becomes

$$[A^\mu(\vec{x},t), \dot{A}^\nu(\vec{y},t)] = -ig^{\mu\nu}\delta(\vec{x}-\vec{y}) \ . \tag{1.299}$$

This commutation relation can be compared with the one for the uncharged Klein–Gordon field

$$[\varphi(\vec{x},t), \dot{\varphi}(\vec{y},t)] = i\delta(\vec{x}-\vec{y}) \ , \tag{1.300}$$

From this we see that the spacial components A^i indeed obey normal commutation relations while on the other hand the time component A^0 obeys

$$[A_0(\vec{x},t), \dot{A}_0(\vec{y},t)] = -i\delta(\vec{x}-\vec{y}) \ , \tag{1.301}$$

which is a commutation relation with the wrong sign. Let us now consider the commutation relation of $\partial_\mu A^\mu$ with A^ν:

$$\begin{aligned}
[\partial_\mu A^\mu(\vec{x},t), A^\nu(\vec{y},t)] &= [\partial_0 A^0(\vec{x},t) + \vec{\nabla}\cdot\vec{A}(\vec{x},t), A^\nu(\vec{y},t)] \\
&= -[\pi^0(\vec{x},t), A^\nu(\vec{y},t)] + \vec{\nabla}\cdot[\vec{A}(\vec{x},t), A^\nu(\vec{y},t)] \\
&= ig^{\nu 0}\delta(\vec{x}-\vec{y}) \neq 0 \ .
\end{aligned} \tag{1.302}$$

This means that we cannot impose the Lorentz gauge condition $\partial_\mu A^\mu = 0$ as an operator equation.

But let's forget about these problems for the moment and just naively proceed with canonical quantisation. Just as the Klein–Gordon and Dirac field, we will also expand the Maxwell field A_μ in normal modes (plane waves):

$$A_\mu(\vec{x},t) = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}} \sum_{\lambda=0}^{3} \left[a_\lambda(\vec{k})\epsilon_\mu^\lambda(\vec{k}) e^{i(\vec{k}\cdot\vec{x}-\omega t)} + a_\lambda^\dagger(\vec{k})\epsilon_\mu^\lambda(\vec{k}) e^{-i(\vec{k}\cdot\vec{x}-\omega t)} \right] \ . \tag{1.303}$$

Because $\Box A_\mu = 0$ we have $k^2 = k\cdot k = k_0^2 - |\vec{k}|^2 = 0$, or:

$$\omega(k) = |\vec{k}| \tag{1.304}$$

and we find the dispersion relation of a massles field. Because A^μ is a fourvector, we can decompose for every$\vec{k}$ the Fourier component of A^μ along four linearly independent basis vectors$\epsilon^\mu_\lambda(\vec{k})$. We can choose the de z-axis parallel to $\vec{k}$ and define the independent vectors

$$\epsilon^0_\mu = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \quad , \quad \epsilon^1_\mu = \begin{pmatrix}0\\1\\0\\0\end{pmatrix} \quad , \quad \epsilon^2_\mu = \begin{pmatrix}0\\0\\1\\0\end{pmatrix} \quad , \quad \epsilon^3_\mu = \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \ . \tag{1.305}$$

The physical polarisations are $\lambda = 1, 2$ which are transversal ($\perp \vec{k}$). The polarisation vectors are orthonormal

$$\epsilon^\lambda_\mu \epsilon^{\lambda' \mu} = g^{\lambda\lambda'} \tag{1.306}$$

and form a basis of the real vector space of fourvectors obeying the completeness relation

$$\sum_{\lambda,\lambda'} g_{\lambda\lambda'} \epsilon^\lambda_\mu \epsilon^{\lambda'}_\nu = g_{\mu\nu} \ . \tag{1.307}$$

From the completeness relation and the Fourier representation (1.303) we find that the commutation relations (1.299) and $[A_\mu, A_\nu] = [\dot{A}_\mu, \dot{A}_\nu] = 0$ are fulfilled if

$$[a_\lambda(\vec{k}), a^\dagger_{\lambda'}(\vec{k}')] = -g_{\lambda\lambda'}\delta(\vec{k} - \vec{k}') \tag{1.308a}$$

$$[a_\lambda(\vec{k}), a_{\lambda'}(\vec{k}')] = [a^\dagger_\lambda(\vec{k}), a^\dagger_{\lambda'}(\vec{k}')] = 0 \ . \tag{1.308b}$$

As usual, the vacuum obeys:

$$a_\lambda(\vec{k})|0\rangle = 0 \ . \tag{1.309}$$

A one photon state with momentum $\vec{k}$ and polarisationλ is

$$a^\dagger_\lambda(\vec{k})|0\rangle = |\vec{k}, \lambda\rangle \ . \tag{1.310}$$

These states are normalised as

$$\begin{aligned} \langle \vec{k}', \lambda' | \vec{k}, \lambda\rangle &= \langle 0 | a_{\lambda'}(\vec{k}') a^\dagger_\lambda(\vec{k}) | 0\rangle \\ &= \langle 0 | [a_{\lambda'}(\vec{k}'), a^\dagger_\lambda(\vec{k})] | 0\rangle \\ &= -g_{\lambda\lambda'}\delta(\vec{k} - \vec{k}') \ . \end{aligned} \tag{1.311}$$

From this we conclude that the photons with scalar polarisation ($\lambda = 0$) are described by states that have negative norm. This however is no problem because only the transversal photons ($\lambda = 1, 2$) are physical and they do have a positive norm.

The problem is however that we must be sure that the unphysical polarisations ($\lambda = 0, 3$) do not contribute to physical quantities. Let us take the energy for example. By substitution of the Fourier expansion (1.303) in the Hamiltonian density (**??**) we find after integration over space and using the orthonormality relations for the polarisation vectors:

$$\begin{aligned} H &= \int d^3x(\pi^\mu \dot{A}_\mu - \mathcal{L}) \\ &= \frac{1}{2}\int d^3x \left(\sum_{i=1}^{3} \dot{A}_i^2 + (\vec{\nabla}A_i)^2\right) - \dot{A}_0^2 - (\vec{\nabla}A_0)^2 \\ &= \int d^3k\ \omega(k) \left[\sum_{\lambda=1}^{3} a_\lambda^\dagger(\vec{k})a_\lambda(\vec{k}) - a_0^\dagger(\vec{k})a_0(\vec{k})\right] + E_0\ . \end{aligned} \tag{1.312}$$

We therefore have to take care that the scalar ($\lambda = 0$) and longitudinal ($\lambda = 3$, along $\vec{k}$) polarisations do not contribute to the energy. We can do this by at this stage imposing the Lorentz gauge condition.

Because we cannot impose the gauge condition as an operator identity (this is in conflict with the commutation relations) we will instead impose a condition to the physical state vectors $|\Phi\rangle$ such that the gauge condition is obeyed in the mean:

$$\langle\Phi|\partial_\mu A^\mu|\Phi\rangle = 0\ . \tag{1.313}$$

We can now split the field operator A^μ in a positive frequency part (annihilation part) $A^{\mu(+)}$ and a negative frequency part $A^{\mu(-)}$ (creation part):

$$A^\mu(x) = A^{\mu(+)} + A^{\mu(-)}\ . \tag{1.314}$$

Let us now impose the following linear condition to the physical state vectors$|\Phi\rangle$:

$$\partial_\mu A^{\mu(+)}(\vec{x},t)|\Phi\rangle = 0\ . \tag{1.315}$$

From this it follows by Hermitian conjugation that

$$\langle\Phi|\partial_\mu A^{\mu(-)}(\vec{x},t) = 0 \tag{1.316}$$

so that

$$\langle\Phi|\partial_\mu A^\mu|\Phi\rangle = \langle\Phi|\partial_\mu A^{\mu(+)}|\Phi\rangle + \langle\Phi|\partial_\mu A^{\mu(-)}|\Phi\rangle = 0\ . \tag{1.317}$$

The condition (1.315) has been proposed for the first time in 1950 by S. Gupta and K. Bleuler and is called the Gupta-Bleuler condition. This way of quantising the Maxwell field is called Gupta-Bleuler quantisation. If we substitute the annihilation part of the Fourier expansion of A^μ in (1.315), then the Gupta-Bleuler condition becomes

$$\int \frac{d^3k}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega(k)}} e^{-ik\cdot x} \sum_{\lambda=0}^{3} k\cdot\epsilon_\lambda(\vec{k})a_\lambda(\vec{k})|\Phi\rangle = 0\ . \tag{1.318}$$

Because the $\lambda = 1,2$-polarisations are transversal $(k \cdot \epsilon_\lambda(\vec{k}),\ \lambda = 1,2)$ and $k \cdot \epsilon_0(\vec{k}) = -k \cdot \epsilon_3(\vec{k})$, the Gupta-Bleuler condition (1.318) is fulfilled for all $\vec{k}$ if

$$(a_0(\vec{k}) - a_3(\vec{k}))|\Phi\rangle = 0 \tag{1.319}$$

and hence also

$$\langle\Phi|(a_0^\dagger(\vec{k}) - a_3^\dagger(\vec{k})) = 0\ . \tag{1.320}$$

From this it follows that

$$\langle\Phi|a_0^\dagger(\vec{k})a_0(\vec{k})|\Phi\rangle = \langle\Phi|a_3^\dagger(\vec{k})a_3(\vec{k})|\Phi\rangle\ , \tag{1.321}$$

so that a physical state which obeys the Lorentz gauge condition has as many longitudinal $(\lambda = 3)$ as scalar $(\lambda = 0)$ photons. The expectation value of the Hamiltonian (**??**) for a physical state$|\Phi\rangle$ is then:

$$\begin{aligned}
\langle\Phi|H|\Phi\rangle &= \int d^3k\ \omega(k)\sum_{\lambda=1}^{2}\langle\Phi|a_\lambda^\dagger(\vec{k})a_\lambda(\vec{k})|\Phi\rangle + \int d^3k\ \omega(k)\langle\Phi a_3^\dagger(\vec{k})a_3(\vec{k}) - a_0^\dagger(\vec{k})a_0(\vec{k})|\Phi\rangle \\
&= \int d^3k\ \omega(k)\sum_{\lambda=1}^{2}\langle\Phi|n(\vec{k},\lambda)|\Phi\rangle
\end{aligned} \tag{1.322}$$

with $n(\vec{k},\lambda)$ the number of photons with polarisation λ. The unphysical polarisations give no contribution to the total energy. One can show that this is also true for other physical (gauge invariant) quantities. The unphysical polarisation also do not contribute to the norm of a physical state $|\Phi\rangle$ because the scalar photons give as many negative contributions as the longitudinal photons give positive ones so that they perfectly compensate each other in the norm:

$$\langle\Phi|\Phi\rangle \geq 0\ . \tag{1.323}$$

The physical states belong to a positive definite subspace of the total Hilbert space, defined by the Gupta-Blueler condition. This is typical for the quantisation of massless particles of spin 1 (photons, gauge bosons) and spin 2 (gravitons) if one wants to do it in a manifestly covariant way. In this case one always needs a bigger Hilbert space which is not positive definite and which one has to restrict by imposing a gauge condition on the states. For the quantisation of non-abelian gauge bosons,for example, one not only has the unphysical polarisations of the gauge bosons but on also has to introduce the so called Faddeev-popov ghosts which are unphysical scalar particles which obey Fermi statistics and don't obey the spin statistics theorem. In this case one has to generalise the Gupta-Bleueler formalism.