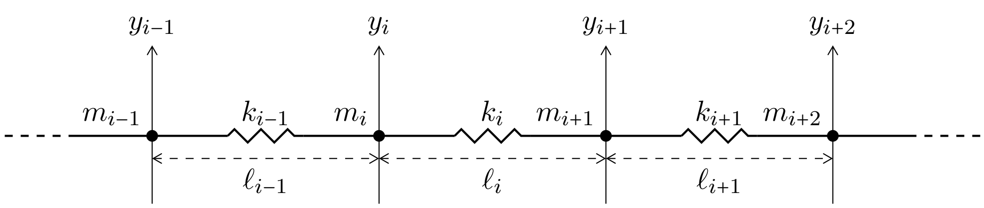
Chapter 2

Field Quantization

2.1 Classical Fields

Consider a (classical, non-relativistic) system of masses, m_i, connected by springs, so that m_i and m_{i+1} are connected by a spring with spring constat k_i. In equilibrium the masses all lie on a straight line, and the distance between masses m_i and m_{i+1} is ℓ_i. The masses are free to move only on a fixed direction perpendicular to this straight line. This is shown in the figure below. We are free to use a



coordinate system to describe the positions of the masses with the x-axis along the equilibrium straight line and the y-axis the transverse direction in which the masses are constrained to move. The i-th mass has coordinates $\vec{x}_i$. To describe the dynamics of this system we construct the Lagrangian,

$$L = L(\dot{y}_i, y_i) = \sum_i \tfrac{1}{2} m_i \dot{y}_i^2 - V(|\vec{x}_{i+1} - \vec{x}_i|)$$

where

$$V = \sum_i \tfrac{1}{2} k_i |\vec{x}_{i+1} - \vec{x}_i|^2 = \tfrac{1}{2} k_i \left((y_{i+1} - y_i)^2 + \ell_i^2 \right)$$

so that, dropping the irrelevant constant

$$L = L(\dot{y}_i, y_i) = \sum_i \tfrac{1}{2} m_i \dot{y}_i^2 - \tfrac{1}{2} k_i (y_{i+1} - y_i)^2 \,.$$

We are interested in this system in the limit that we cannot resolve the individual masses, so by our measuring apparatus the system appears as a continuum. Mathematically we want to take the limit $\ell_i \to 0$ and describe the displacement of the system from the x-axis at some point x along the axis, at time t, by a function $\xi(x,t)$. This function is called a *field*. Since the displacement is y_i at position x_i along the axis, we identify $y_i(t) \to \xi(x_i,t)$. Note that while x_i is used classically as a coordinate of a particle, in $\xi(x,t)$ it is just a label telling us where we are measuring the displacement ξ. This is an important point, so I dwell on it a bit, since first time students of quantum field theory often get confused with the role of x in the argument of a field. The field value itself can be measuring something other than displacement. For example, it could be temperature or pressure, or electric field. The argument x, or in the three-dimensional case $\vec{x}$ of a field indicates where the field has a particular value. So x (or $\vec{x}$) is not a dynamical variable, but ξ is.

To rewrite the Lagrangian in terms of the field, use

$$y_{i+1} - y_i \to \xi(x_i + \ell_i, t) - \xi(x_i, t) = \ell_i \left.\frac{\partial \xi}{\partial x}\right|_{x=x_i} + \cdots,$$

where the ellipses stand for terms with higher powers of ℓ_i, and $\dot{y}_i \to \left.\frac{\partial \xi}{\partial t}\right|_{x=x_i}$. Multiplying and dividing by ℓ_i and interpreting $\ell_i = x_{i+1} - x_i$ as the Δx, we have then

$$L = \sum_i \Delta x \left[\frac{1}{2}\frac{m_i}{\ell_i}\left(\frac{\partial \xi}{\partial t}\right)^2 - \frac{1}{2}k_i\ell_i\left(\frac{\partial \xi}{\partial x}\right)^2 \right]$$

where the derivatives are evaluated at $x = x_i$. We take the limit $\ell_i \to 0$ keeping the ratio m_i/ℓ_i and the product $k_i\ell_i$ finite. These fixed ratio and product then can be characterized with functions $\sigma(x)$ and $\kappa(x)$ (with $\sigma(x_i) = m_i/\ell_i$ and $\kappa(x_i) = k_i\ell_i$ in the limiting process. Of course, the sum becomes an integral and we have

$$L = \int dx\, \mathcal{L} = \int dx \left[\frac{1}{2}\sigma(x)\left(\frac{\partial \xi}{\partial t}\right)^2 - \frac{1}{2}\kappa(x)\left(\frac{\partial \xi}{\partial x}\right)^2 \right].$$

The function $\mathcal{L} = \mathcal{L}(\partial_t\xi, \partial_x\xi, \xi, x, t)$ is called a *Lagrangian density*. This is our first example of a field theory. The dynamics of the field $\xi(x,t)$ is specified by the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\sigma(x)\left(\frac{\partial \xi}{\partial t}\right)^2 - \frac{1}{2}\kappa(x)\left(\frac{\partial \xi}{\partial x}\right)^2 .$$

In no time we will get tired of saying “Lagrangian density” so, as is commonly done in practice, we will improperly refer to $\mathcal{L}$ as a Lagrangian. The distinction should be clear from the context (if it is integrated it is actually a Lagrangian, else it is a density). It should be no surprise that a dynamical variable that varies continuously in space requires densities for its description.

We are often interested in systems that are homogeneous in space, that is, the location of the origin of the coordinate system should be irrelevant. So we impose that the Lagrangian be invariant under a space translation $x' = x - a$. The fields change into new fields $\xi'(x', t) = \xi(x, t)$, which is just a relabeling of the dynamical variables (a canonical transformation, to be precise). But $\sigma(x)$ and $\kappa(x)$ do change, unless $\sigma(x+a) = \sigma(x)$ and $\kappa(x+a) = \kappa(x)$ for any a. This implies, $\sigma(x) = \sigma =$ constant and $\kappa(x) = \kappa =$ constant. Given this, it is convenient to introduce a change of variables, $\phi(x,t) = \sqrt{\kappa}\xi(x,t)$, so that the Lagrangian density is written more simply:

$$\mathcal{L} = \frac{1}{2}\frac{1}{c_s^2}\left(\frac{\partial\phi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 . \tag{2.1}$$

where we have introduced the shorthand $c_s^2 = \kappa/\sigma$.

Before we go over to find the equations of motion for this system, let's review the derivation of the Euler-Lagrange equations (or *equations of motion*) for a system with discrete degrees of freedom. Given a Lagrangian $L = L(\dot{q}^a, q^a)$, Hamilton's principle says the equations of motion are obtained from requiring that the action integral be extremized:

$$\delta S[q^a(t)] = \delta \int_{t_1}^{t_2} dl\, L(\dot{q}^a, q^a) = 0 \qquad \text{with} \quad q^a(t_1) = q^a_{\text{ini}} \text{ and } q^a(t_2) = q^a_{\text{fin}}$$

Computing we have,

$$0 = \int_{t_1}^{t_2} dt \sum_a \left[\frac{\partial L}{\partial \dot{q}^a}\frac{d}{dt}\delta q^a + \frac{\partial L}{\partial q^a}\delta q^a\right] = \int_{t_1}^{t_2} dt \sum_a \delta q^a \left[-\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^a} + \frac{\partial L}{\partial q^a}\right] + \left.\frac{\partial L}{\partial \dot{q}^a}\delta q^a\right|_{t_1}^{t_2}$$

The last term vanishes by the fixed boundary conditions $\delta q^a(t_{1,2}) = 0$, and the first term vansihes for arbitrary variation $\delta q^a(t)$ if

$$\frac{\partial L}{\partial q^a} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^a} + = 0$$

These are the Euler-Lagrange equations.

Moving on to the continuum case, we apply the same principle, that the action integral be an extremum under variations of the dynamical variable, $\phi(x,t)$:

$$\delta S[\phi(x,t)] = \delta \int dt L = \delta \int_{t_1}^{t_2} dt \int dx \mathcal{L}(\partial_t\phi, \partial_x\phi, \phi, t) = 0.$$

The boundary conditions are now $\phi(x, t_1) = \phi_{\text{ini}}(x)$ and $\phi(x, t_2) = \phi_{\text{fin}}(x)$. We have intentionally not specified boundary conditions for the x-integration. This will allow us to decide what are reasonable conditions as we derive equations of motion. Computing the variation of S does not introduce new complications:

$$
\begin{aligned}
0 = \delta S &= \int_{t_1}^{t_2} dt \int dx \left[\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial t}\right)} \frac{\partial\delta\phi}{\partial t} + \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial x}\right)} \frac{\partial\delta\phi}{\partial x} + \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi \right] \\
&= \int_{t_1}^{t_2} dt \int dx \delta\phi \left[-\frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial t}\right)} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial x}\right)} + \frac{\partial\mathcal{L}}{\partial\phi} \right] \\
&\qquad + \int dx \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial t}\right)} \delta\phi\Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial x}\right)} \delta\phi\Big|_{x=?}
\end{aligned}
$$

The first term on the last line vanishes by the boundary conditions at $t = t_{1,2}$. The second term vanishes if we fix boundary conditions on $\phi(x,t)$ at the limits of integration for x. If the field is defined over the whole line $x \in (-\infty,\infty)$ then we can specify $\lim_{x\to\pm\infty} \phi(x,t) = 0$. This is reasonable. If you start with the collection of springs and masses form its equilibrium configuration, and poke it somewhere, it will take infinite time for the masses infinitely far away to be excited. But we are considering finite time, and in finite time the masses far away never get displaced from equilibrium. This is even clearer in the continuum case. We will see shortly that ϕ satisfies a wave equation with finite speed of propagation. Alternatively, we can imagine the case of a finite system of springs and masses extending from $x = 0$ to $x = L$. The limit of $\ell_i \to 0$ still requires that we take the number of masses and springs to infinity, but we can do so with the field confined to the region $x \in [0, L]$. In this case we need to introduce boundary conditions at $x = 0$ and L. If the ends of the line of masses are fixed, then in the limit $\phi(0,t)$ $\phi(L,t)$ are fixed. Another popular setup is to have periodic boundary conditions, $\phi(L,t) = \phi(0,t)$. This means the field is defined on a 1-dimensional torus (really a circle, but the generalization to higher dimensions is a torus). This also makes the last terms vanish. Physically, if we have only finite time and the size of the system L is sufficiently large, the precise choice of boundary conditions should be irrelevant.

Setting to zero the coefficient of the arbitrary variation $\delta\phi(x,t)$ gives the Euler-Lagrange equations:

$$
-\frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial t}\right)} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial x}\right)} + \frac{\partial\mathcal{L}}{\partial\phi} = 0\,,
$$

To obtain equations of motion in our example, (2.1), compute,

$$
\frac{\partial\mathcal{L}}{\partial\phi} = 0\,, \qquad \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial x}\right)} = -\frac{\partial\phi}{\partial x}\,, \qquad \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial\phi}{\partial t}\right)} = \frac{1}{c_s^2}\frac{\partial\phi}{\partial t}\,,
$$

and use in the Euler-Lagrange equations:

$$\boxed{\frac{1}{c_s^2}\frac{\partial^2\phi}{\partial t^2} - \frac{\partial^2\phi}{\partial x^2} = 0}$$

You recognize this as the wave equation! The general solution is

$$\phi_R(x - c_s t) + \phi_L(x + c_s t)$$

describing right and left moving waves with speed of propagation c_s (the speed of "sound," hence the subscript s).

Since the notation above is pretty unwieldy, we use, as previously advertised, ∂_t for $\partial/\partial t$, and ∂_x for $\partial/\partial x$ so that, for example, we write the Euler-Lagrange equations as

$$-\partial_t \frac{\partial\mathcal{L}}{\partial_t\phi} - \partial_x \frac{\partial\mathcal{L}}{\partial_x\phi} + \frac{\partial\mathcal{L}}{\partial\phi} = 0\,.$$

Relativistic Fields In the example above we are free to take the speed of light $c = 1$ for the parameter c_s. The solutions to the equation of motion are waves that propagate at the speed of light. Is this then a Lorentz invariant theory? Yes!

We can check this by verifying that if $\phi(x,t)$ is a solution, so is $\phi'(x,t) \equiv \phi(x',t')$ where

$$\begin{aligned} x' &= \gamma(x - \beta t) \\ t' &= \gamma(t - \beta x) \end{aligned} \qquad\qquad \gamma = \frac{1}{\sqrt{1-\beta^2}}$$

Alternatively, we can verify that the action integral , $S = \int\int \mathcal{L}\, dt\, dx$, from which the equations are derived, is itself invariant. To this end compute,

$$\begin{aligned}
\frac{\partial\phi'(x,t)}{\partial x} &= \frac{\partial\phi(x',t')}{\partial x} = \frac{\partial\phi(x',t')}{\partial x'}\frac{\partial x'}{\partial x} + \frac{\partial\phi(x',t')}{\partial t'}\frac{\partial t'}{\partial x} = \gamma\frac{\partial\phi(x',t')}{\partial x'} - \beta\gamma\frac{\partial\phi(x',t')}{\partial t'} \\
\frac{\partial\phi'(x,t)}{\partial t} &= \frac{\partial\phi(x',t')}{\partial x} = \frac{\partial\phi(x',t')}{\partial x'}\frac{\partial x'}{\partial t} + \frac{\partial\phi(x',t')}{\partial t'}\frac{\partial t'}{\partial t} = -\beta\gamma\frac{\partial\phi(x',t')}{\partial x'} + \gamma\frac{\partial\phi(x',t')}{\partial t'}
\end{aligned}$$

and use this in the Lagrangian density, (2.1) (with $c_s = c = 1$):

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\phi'(x,t)}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi'(x,t)}{\partial x}\right)^2 = \frac{1}{2}\left(\frac{\partial\phi(x',t')}{\partial t'}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi(x',t')}{\partial x'}\right)^2\,.$$

Finally integrate this over $\int\int dtdx$ to obtain the action. On the right hand side of the equation change variables of integration , $dx\,dt = \left|\frac{\partial(x,t)}{\partial(x',t')}\right| dx'\,dt' = dx'\,dt'$ to obtain finally

$$\int\int dt\,dx\,\mathcal{L}(\phi'(x,t)) = \int\int dt'\,dx'\,\mathcal{L}(\phi(x',t')) = \int\int dt\,dx\,\mathcal{L}(\phi(x,t))$$

where in the last step we changed the label for the dummy variables of integration from (x', t') to (x, t). This shows invariance of the action integral, $S[\phi'(x,t)] = S[\phi(x,t)]$; the theory is Lorentz invariant.

We could have saved ourselves a lot of time had we taken advantage of the notation designed to exhibit the properties of quantities under Lorentz transformations. We can rewrite the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\phi(x,t)}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi(x,t)}{\partial x}\right)^2 = \frac{1}{2}\eta^{\mu\nu}\,\partial_\mu\phi\,\partial_\nu\phi = \frac{1}{2}\partial^\mu\phi\partial_\mu\phi$$

As we have seen $\partial_\mu\phi$ transforms as a vector, and the Lagrangian is just the invariant square of this vector!

Klein-Gordon, again While the Lagrangian density above was obtained by a limiting process from a system fo discrete masses and springs, we do not insist in interpreting the relativistic system as some collection of infinitesimal springs and masses. We can take a more general approach to writing a Lagrangian density which may be a good model for some physical system by insisting it written in terms of the appropriate number and type of fields, and constraining it by principles and symmetries we want to incorporate.

For example: Suppose we have a system in 1-spatial dimension that can be described by a single field, $\phi(x,t)$. Moreover, we want it to satisfy an equation of motion of second order (no more than second time derivatives), and we want the action to be invariant under Lorentz transformations. Then the Lagrangian density, $\mathcal{L} = \mathcal{L}(\phi, \partial_\mu\phi)$, can include derivatives only through the invariant $\partial^\mu\phi\partial_\mu\phi$. The simplest Lagrangian density we can think of is the one in the example above, $\mathcal{L} = \frac{1}{2}\partial^\mu\phi\partial_\mu\phi$. The next simplest is

$$\mathcal{L} = \tfrac{1}{2}\partial^\mu\phi\partial_\mu\phi - \tfrac{1}{2}m^2\phi^2.$$

We could have included also a linear term, $g\phi$, with g a a constant, but we can eliminate that term by a field redefinition $\phi \to \phi + g/m^2$. The Euler-Lagrange equation that follows from this Lagrangian density is the 1-spatial dimension version of the Klein-Gordon equation! It is instructive to derive the equation of motion anew, maintaing Lorentz covariance explicitly throughout the computation. We first integrate by parts to recast the action as

$$S[\phi] = \int d^2x\,\left[-\tfrac{1}{2}\phi\partial^2\phi - \tfrac{1}{2}m^2\phi^2\right]$$

where $\partial^2 = \partial^\mu\partial_\mu$. Taking a variation is now trivial,

$$0 = \delta S = -\int d^2x\,\delta\phi\left[\partial^2\phi + m^2\phi\right]$$

leading to

$$\left(\partial^2 + m^2\right)\phi(x,t) = 0$$

which you recognize as the Klein-Gordon equation.

2.2 Field Quantization

As we argued in the introduction we need to account for pair creation not just because it is a natural phenomena and because it matters for accuracy, but also because it is required if we are to have a consistent relativistic quantum mechanical theory. We could proceed by enlarging the Hilbert space to include multi-particle states, $|\vec{p}\rangle$, $|\vec{p},\vec{p}\,'\rangle = |\vec{p}\rangle \otimes |\vec{p}\,'\rangle$, etc, and then introduce creation/annihilation operators to describe interactions that change particle number. The end result is the same as what we will obtain from tackling head on the problem of quantization of fields.

Before we do so, let's review quantization of classical systems with a discrete set of generalized coordinates q_i, with $i = 1,\ldots,N$. We are given a Lagrangian, from which conjugate momenta and a Hamiltonian follow:

$$L = L(q_i,\dot{q}_i) \quad \Rightarrow \quad p_i = \frac{\partial L}{\partial \dot{q}_i} \quad \text{and} \quad H = p_i\dot{q}_i - L$$

Poisson brackets are defined on any functions of p_i and q_i by

$$\{f,g\}_P = \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i}\frac{\partial f}{\partial p_i}. \tag{2.2}$$

Note that here, and in the definition of the Hamiltonian, we have used the generalized Einstein summation convention. One has, in particular, $\{q_i,p_j\}_P = \delta_{ij}$ and $\{q_i,q_j\}_P = 0 = \{p_i,p_j\}_P$. Moreover, the equations of motion in the Hamiltonian formalism can be written as $\dot{p}_j = \{p_j,H\}_P = -\partial H/\partial q_j$ and $\dot{q}_j = \{q_j,H\}_P = \partial H/\partial p_j$. Quantization proceeds by associating an operator on a Hilbert space $\mathcal{H}$ with each of the generalized coordinates and momenta, $q_i \to \hat{q}_i$ and $p_i \to \hat{p}_i$, and replacing the Poisson bracket by ($-i$ times) the commutator of the operators, $\{q_i,p_j\}_P = \delta_{ij} \to -i[\hat{q}_i,\hat{p}_j] = \delta_{ij}$. Similarly $[\hat{q}_i,\hat{q}_j] = 0 = [\hat{p}_i,\hat{p}_j]$. Evolution of operators is given likewise, e.g., $i\dot{\hat{p}}_j = [\hat{p}_j,\hat{H}]$ and $i\dot{\hat{q}}_j = [\hat{q}_j,\hat{H}]$.

We would like to use this same method to quantize field theories. Let's first understand the analogues of conjugate momentum, Hamiltonian and Poisson bracket in classical field theory and only then quantize. Consider the 1-spatial dimensional system of the previous section. How do we take the continuum limit of the Poisson brackets, Eq. (2.2)? It is convenient to start with

$$\sum_j \{q_i,p_j\}_P = \sum_j \delta_{ij} = 1$$

For the continuum limit rewrite $\sum_j p_j = \sum_j \ell(p_j/\ell)$, where we have taken a common separation $\ell_i = \ell$ for simplicity. This suggests $p_j(t) \to \pi(x,t)$, some sort of conjugate momentum density. On the right hand side of the Poisson bracket then $1 = \sum_j \delta_{ij} \to \int dx\, \delta(x-x')$. That is

$$\{\phi(x), \pi(x')\}_P = \delta(x-x')$$

Since

$$\frac{\delta\phi(x)}{\delta\phi(x')} = \delta(x-x')$$

we are led to define

$$\{f,g\}_P = \int dx \left[\frac{\delta f}{\delta\phi(x)}\frac{\delta g}{\delta\pi(x)} - \frac{\delta g}{\delta\phi(x)}\frac{\delta f}{\delta\pi(x)}\right]$$

The momentum conjugate to ϕ can be defined intrinsically (without taking a limit of the discrete system),

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

and the Hamiltonian *density* is defined by

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

We are ready to quantize this 1+1 dimensional field theory. We introduce hermitian operators $\hat\phi$ and $\hat\pi$ on a Hilbert space, and use the quantization prescription that gives us commutation relations from the Poisson brackets,

$$-i[\hat\phi(x,t), \hat\pi(x',t)] = \delta(x-x')\,, \qquad [\hat\phi(x,t), \hat\phi(x',t)] = 0 = [\hat\pi(x,t), \hat\pi(x',t)] \tag{2.3}$$

Note that the commutation relations are given at a common time, but separate space coordinate. The field operators satisfy equations of motion, the Euler-Lagrange equations from the Lagrangian density $\mathcal{L}$. Alternatively, time evolution is given by

$$i\partial_t\hat\pi(x,t) = [\hat\pi(x,t), \hat H] \quad \text{and} \quad i\partial_t\hat\phi(x,t) = [\hat\phi(x,t), \hat H]$$

where the Hamiltonian is

$$\hat H = \int dx\, \hat{\mathcal{H}}\,.$$

Let's work this out for the 1+1 Klein-Gordon example:

$$\mathcal{L} = \tfrac{1}{2}\partial^\mu\hat\phi\partial_\mu\hat\phi - \tfrac{1}{2}m^2\hat\phi^2\,.$$

The momentum conjugate to $\hat\phi$ is

$$\hat\pi = \frac{\partial\mathcal{L}}{\partial\dot\phi} = \partial_t\hat\phi$$

and the Hamiltonian density is

$$\hat{\mathcal{H}} = \tfrac{1}{2}\hat{\pi}^2 + \tfrac{1}{2}(\partial_x\hat{\phi})^2 + \tfrac{1}{2}m^2\hat{\phi}^2 \,.$$

The quantum field equation is just the Klein-Gordon equation,

$$[\partial^2 + m^2]\hat{\phi}(x,t) = 0 \,.$$

Alternatively,

$$i\partial_t\hat{\pi}(x,t) = [\hat{\pi}(x,t),\hat{H}] = -i(-\partial_x^2\hat{\phi}+m^2\hat{\phi}) \quad \text{and} \quad i\partial_t\hat{\phi}(x,t) = [\hat{\phi}(x,t),\hat{H}] = i\hat{\pi}(x,t)$$

The fields satisfy the equal-time commutation relations (2.3). To understand the content of this theory, we Fourier expand, at fixed time, say $t = 0$

$$\hat{\phi}(x) = \int \frac{dk}{2\pi}\widetilde{\phi}(k)e^{ikx} \qquad \text{and} \qquad \hat{\pi}(x) = \int \frac{dk}{2\pi}\widetilde{\pi}(k)e^{ikx}.$$

That $t = 0$ is implicit here and in the next few lines. Since $\hat{\phi}^\dagger(x) = \hat{\phi}(x)$ we have $\widetilde{\phi}(k)^\dagger = \widetilde{\phi}(-k)$ and $\widetilde{\pi}(k)^\dagger = \widetilde{\pi}(-k)$. The equal-time commutation relations $[\hat{\phi}(x),\hat{\phi}(x')] = 0$ and $[\hat{\pi}(x),\hat{\pi}(x')] = 0$ imply

$$[\widetilde{\phi}(k),\widetilde{\phi}(k')] = 0 = [\widetilde{\pi}(k),\widetilde{\pi}(k')]$$

Then $[\hat{\phi}(x),\hat{\pi}(x')] = i\delta(x-x')$ gives

$$i\delta(x-x') = \int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\left[\widetilde{\phi}(k)e^{ikx},\widetilde{\pi}(k')e^{ik'x'}\right] \Rightarrow [\widetilde{\phi}(k),\widetilde{\pi}(k')] = 2\pi i\delta(k+k')$$

The advantage of Fourier transforming shows up first in computing the Hamiltonian, since the ∂_x^2 term is diagonalized:

$$\begin{aligned}\hat{H} &= \int \frac{dk}{2\pi}\left[\tfrac{1}{2}\widetilde{\pi}^\dagger(k)\widetilde{\pi}(k) + \tfrac{1}{2}(k^2+m^2)\widetilde{\phi}^\dagger(k)\widetilde{\phi}(k)\right] \\ &= \int \frac{dk}{2\pi}\left[\tfrac{1}{2}\widetilde{\pi}^\dagger(k)\widetilde{\pi}(k) + \tfrac{1}{2}\omega_k^2\widetilde{\phi}^\dagger(k)\widetilde{\phi}(k)\right]\end{aligned}$$

I have written ω_k for the energy $\omega_k = E_k = \sqrt{k^2+m^2}$ for two reasons: (i) we have not shown that k is a momentum so we have no right yet to think of $\sqrt{k^2+m^2}$ as the energy, and (ii) it becomes clear that the expression for H is that of an infinite sun of linear harmonic oscillators, $\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{q}^2$.

Review of QM-simple harmonic oscillator Consider the spring mass system described by

$$L = \tfrac{1}{2}\dot{q}^2 - \tfrac{1}{2}\omega^2 q^2$$

Correspondingly

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2 q^2$$

Here q and p, aas well as H, are operators on the Hilbert space, but we are suppressing the hat over the symbols since there will be no occasion for confusion:

$$i[p, q] = 1$$

Let

$$a = \frac{1}{\sqrt{2\omega}}(\omega q + ip)$$
$$a^\dagger = \frac{1}{\sqrt{2\omega}}(\omega q - ip)$$

Then $a^\dagger a = 1/2\omega(\omega^2 q^2 + p^2 - i\omega[p, q]) = 1/2\omega(2H - \omega)$ or

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

Moreover, $[a, a^\dagger] = \frac{1}{2\omega}[\omega q + ip, \omega q - ip] = \frac{1}{2\omega}(2i\omega)[p, q]$ so we have

$$[a, a^\dagger] = 1$$
$$[a, a] = 0$$
$$[a^\dagger, a^\dagger] = 0$$

and then

$$[H, a^\dagger] = \omega a^\dagger$$
$$[H, a] = -\omega a$$

We can use these to find the spectrum. Assume that the state $|E\rangle$ is an energy eigenstate:

$$H|E\rangle = E|E\rangle$$

Then

$$H(a^\dagger|E\rangle) = (E + \omega)\left(a^\dagger|E\rangle\right)$$

which means $|E+\omega\rangle = N_+ a^\dagger|E\rangle$ for some normalization constant, N_+. If $|E\rangle$ is normalized, $\langle E|E\rangle = 1$, then

$$\begin{aligned}1 = \langle E+\omega|E+\omega\rangle &= |N_+|^2\langle E|aa^\dagger|E\rangle \\ &= |N_+|^2\langle E|\left([a,a^\dagger] + a^\dagger a\right)|E\rangle \\ &= |N_+|^2\langle E|\left(1 + \frac{1}{2\omega}(2H-\omega) + a^\dagger a\right)|E\rangle \\ &= |N_+|^2\left(\frac{E}{\omega} + \frac{1}{2}\right)\end{aligned}$$

Similarly, $|E-\omega\rangle = N_- a|E\rangle$ and

$$1 = \langle E-\omega|E-\omega\rangle = |N_-|^2\langle E|a^\dagger a|E\rangle = |N_-|^2\left(\frac{E}{\omega} + \frac{1}{2}\right)$$

So we have an infinite tower of states with energies E, $E\pm\omega$, $E\pm 2\omega, \ldots$ Since the operators $a^\dagger$ and a raise and lower energies, we call them raising and lowering operators, respectively. To avoid a spectrum that is unbounded from below (a catastrophic instability once the system is coupled to external forces), we can insist that for some state $|0\rangle$ the tower stops:

$$a|0\rangle = 0$$

This is the minimum energy state, the "ground state." It has energy $H|0\rangle = \frac{1}{2}\omega|0\rangle$, called the "zero-point" energy. Then $a^\dagger|0\rangle$ has energy $E_1 = \omega + \frac{\omega}{2}$ and so on, $(a^\dagger)^n|0\rangle$ has energy $E_n = \omega(n+\frac{1}{2})$. The tower of states then can be labeled by an integer, $|E_n\rangle = |n\rangle$. We assume they are normalized. Then, from above, $|n+1\rangle = N_+ a^\dagger|n\rangle$ with

$$|N_+|^{-2} = \frac{E_n}{\omega} + \frac{1}{2} = n+1$$

so that

$$|n+1\rangle = \frac{1}{\sqrt{n+1}}a^\dagger|n\rangle = \frac{1}{\sqrt{(n+1)n}}(a^\dagger)^2|n-1\rangle = \cdots = \frac{1}{\sqrt{(n+1)!}}(a^\dagger)^{n+1}|0\rangle$$

Note that since $aa^\dagger = a^\dagger a + 1$ one has $\frac{1}{2}\omega(aa^\dagger + a^\dagger a) = \frac{1}{2}\omega(2a^\dagger a + 1) = H$. This way of writing $H = \frac{1}{2}\omega(aa^\dagger + a^\dagger a)$ hides the zero-point energy.

2.2.1 Particle Interpretation

This suggests introducing

$$\begin{aligned}a_k &= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega_k}}\left(\omega_k\widetilde{\phi}(k) + i\widetilde{\pi}(k)\right) \\ a_k^\dagger &= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega_k}}\left(\omega_k\widetilde{\phi}(k)^\dagger - i\widetilde{\pi}(k)^\dagger\right)\end{aligned} \tag{2.4}$$

These have

$$\begin{aligned} [a_k, a_{k'}^\dagger] &= \delta(k-k') \\ [a_k, a_{k'}] &= 0 \\ [a_k^\dagger, a_{k'}^\dagger] &= 0 \end{aligned} \tag{2.5}$$

where we have used $\omega_{-k} = \omega_k$. To compute the Hamiltonian, note that

$$a_k^\dagger a_k = \frac{1}{4\pi\omega_k}\left(\omega_k^2 \widetilde{\phi}(k)^\dagger \widetilde{\phi}(k) + \widetilde{\pi}(k)^\dagger \widetilde{\pi}(k) - i\omega_k \widetilde{\pi}(k)^\dagger \widetilde{\phi}(k) + i\omega_k \widetilde{\phi}(k)^\dagger \widetilde{\pi}(k)\right) . \tag{2.6}$$

Since we are going to sum over $\int dk$, we can change variables $k \to -k$ in the last term,

$$\frac{1}{4\pi\omega_k} i\omega_k \widetilde{\phi}^\dagger(k)\widetilde{\pi}(k) \to \frac{i}{4\pi}\widetilde{\phi}^\dagger(-k)\widetilde{\pi}(-k) = \frac{i}{4\pi}\widetilde{\phi}(k)\widetilde{\pi}(-k)$$

The first two terms in (2.6) are the Hamiltonian density and the last two combine into a commutator, so we have

$$\begin{aligned} \hat{H} &= \frac{1}{2}\int \frac{dk}{2\pi}\left(\widetilde{\pi}(k)^\dagger \widetilde{\pi}(k) + \omega_k^2 \widetilde{\phi}(k)^\dagger \widetilde{\phi}(k)\right) \\ &= \frac{1}{2}\int \frac{dk}{2\pi}\left(4\pi\omega_k a_k^\dagger a_k + \omega_k i[\widetilde{\pi}(k)^\dagger, \widetilde{\phi}(k)]\right) \\ &= \int dk \left(\omega_k a_k^\dagger a_k + \omega_k \delta(0)\right) \\ &= \frac{1}{2}\int dk \omega_k \left(a_k^\dagger a_k + a_k a_k^\dagger\right) \end{aligned}$$

Let's examine what we have. Assuming that there is a ground state such that $a_k|0\rangle = 0$ for all k, we have a Hilbert space obtained by acting with $a_k^\dagger$'s on $|0\rangle$, e.g.,

$$(a_{k_1}^\dagger)^{n_1}(a_{k_2}^\dagger)^{n_2}\cdots)|0\rangle . \tag{2.7}$$

The ground state $|0\rangle$ has energy E_0 given by

$$\hat{H}|0\rangle = \int dk'\, \omega_{k'}\left(a_{k'}^\dagger a_{k'} + \delta(0)\right)|0\rangle = \int dk'\, \omega_{k'}\delta(0)|0\rangle \equiv E_0|0\rangle ,$$

and the state $|k\rangle = a_k^\dagger|0\rangle$ has energy

$$\hat{H}|k\rangle = \int dk'\, \omega_{k'}\left(a_{k'}^\dagger a_{k'} + \delta(0)\right)|k\rangle = (\omega_k + E_0)|k\rangle$$

While the zero-point energy, E_0, is infinite, the difference of energy between the state $|k\rangle$ and the ground state is well defined, finite, $\Delta E = \omega_k$. The same is true of the energy of any of the states (2.7). We can only measure energy differences (except in gravitation; that's another story). That is, we are free to add a constant to H without changing the physical content of the theory. So we can redefine

$$\hat{H} = \int dk\, \omega_k a_k^\dagger a_k$$

Examining this more closely write

$$\hat{H} = \frac{1}{2}\int dk\, \omega_k \left(a_k^\dagger a_k + a_k a_k^\dagger - \langle 0|a_k^\dagger a_k + a_k a_k^\dagger|0\rangle\right) = \int dk\, \omega_k a_k^\dagger a_k\,.$$

We say that in the new expression the operators $a_k^\dagger$ and a_k appear "normal ordered" and the operation is called "normal ordering" or "Wick ordering:"

$$:\tfrac{1}{2}(a_k^\dagger a_k + a_k a_k^\dagger): \equiv a_k^\dagger a_k\,.$$

Under $:\xi:$ the operators in ξ commute. The computation above uses the ground state for reference. We will need to make sure that this procedure preserves Lorentz invariance. More on this later.

The energy of the state $|k\rangle$ is $E_k = \omega_k = \sqrt{k^2+m^2}$. So we identify $p = k$ the momentum of the state. This is just as in our introductory presentation of relativistic QM for a single non-interacting particle. This is then interpreted as a single particle state. But now the theory is much richer. For one thing we have many other states, as in (2.7). The Hilbert space of states in (2.7) is called a "Fock space." We interpret them as many particle states. To see this we check a few things:

(i) Energy of $(a_{k_1}^\dagger)^{n_1}(a_{k_2}^\dagger)^{n_2}\cdots|0\rangle$ is $E = n_1E_{k_1} + n_2E_{k_2} + \cdots$

(ii) Momentum of $(a_{k_1}^\dagger)^{n_1}(a_{k_2}^\dagger)^{n_2}\cdots|0\rangle$ is $p = n_1k_1 + n_2k_2 + \cdots$

The first one follows trivially from the expression for $\hat{H}$ and its action on the states in (2.7). For the second we introduce the operator

$$\hat{p} = \int dk\; k\, a_k^\dagger a_k$$

which gives the desired eigenvalues. We will verify this is the momentum operator below.

From now on we call the operators $a_k^\dagger$ and a_k *creation* and *annihilation* operators, respectively, rather than raising and lowering operators, to remind us that they are adding or taking away a particle from a state. The ground state, $|0\rangle$ is particleless, so we call it the *vacuum state* or just the vacuum.

Statistics As promised, that particles are identical is an automatic consequence of QFT. Note that all particles have the same mass. Moreover, the multiple particle states are automatically symmetric. For example, let $|k_1, k_2\rangle = a^\dagger_{k_1} a^\dagger_{k_2}|0\rangle$. Then

$$|k_1, k_2\rangle = a^\dagger_{k_1} a^\dagger_{k_2}|0\rangle = a^\dagger_{k_2} a^\dagger_{k_1}|0\rangle = |k_2, k_1\rangle$$

where we have used the commutation relations (2.5). More generally $|k_1, \ldots, k_n\rangle$ is symmetric under exchange of any k_i's. This is an unexpected surprise! In NR-QM one simply assumes the wave function is symmetric for bosons (Bose-Einstein statistics), anti-symmetric for fermions (Fermi-Dirac statistics), and it is observed empirically that integer-spin particles are bosons while half-integer spin particles are fermions. There was a hidden assumption in our calculation that resulted in bosonic particles. The assumption is that quantization goes through the replacement $p, q_P \to i[\hat{p}, \hat{q}]_- = i(\hat{p}\hat{q} - \hat{q}\hat{p})$ rather than $p, q_P \to i[\hat{p}, \hat{q}]_+ = i(\hat{p}\hat{q} + \hat{q}\hat{p})$. We will later see that a consistent formulation of QFT requires we use $[\ ,\ ]_-$ for integer spin fields and $[\ ,\ ]_+$ for half-integer spin fields. So not only we will get identical particles automatically, we will get the correct assignment automatically too:

- bosons: spin-0, 1, ...
- fermions: spin-$\frac{1}{2}$, $\frac{3}{2}$, ...

Normalization Note also that

$$\langle k|k'\rangle = \langle 0|a_k a^\dagger_{k'}|0\rangle = \langle 0|[a_k, a^\dagger_{k'}]|0\rangle = \delta(k - k')$$
$$\langle k_1, k_2|k'_1, k'_2\rangle = \langle 0|a_{k_1} a_{k_2} a^\dagger_{k'_1} a^\dagger_{k'_2}|0\rangle = \delta(k_1 - k'_1)\delta(k_2 - k'_2) + \delta(k_1 - k'_2)\delta(k_2 - k'_1)$$

exactly what we expect of identical particle plane wave states. But this is not the desired relativistic normalization. Not a problem, we only need to take for the definition of states

$$|k\rangle = \sqrt{(2\pi)(2E_k)}a^\dagger_k|0\rangle \quad \Rightarrow \quad \langle k|k'\rangle = (2\pi)2E_k\delta(k - k')$$

Plane waves are not normalizable states, but we can make normalizable wave packets out of them:

$$|\psi\rangle = \int dk\, \psi(k) a^\dagger_k|0\rangle \;\Rightarrow\; \langle\psi|\psi\rangle = \int dk\, dk'\, \psi(k)^* \psi(k')\langle 0|a_k a^\dagger_{k'}|0\rangle = \int dk\, |\psi(k)|^2 < \infty$$

It is often convenient to define creation and annihilation operators by rescaling the ones we have:

$$\alpha_k = \sqrt{(2\pi)(2E_k)}a_k$$

so that $|k\rangle = \alpha_k|0\rangle$ has relativistic normalization. In terms of these

$$\hat{H} = \int (dk)\, E_k \alpha_k^\dagger \alpha_k$$
$$\hat{p} = \int (dk)\, k \alpha_k^\dagger \alpha_k$$

where (dk) is the relativistic invariant measure.

Number Operator The state with n-particles is an energy Eigenstate. It therefore evolves into a state with n particles (itself). Particle number is conserved because there are no interactions (yet). This suggest there must be an observable, that is, a hermitian operator, $\hat{N}$ that

(i) is conserved , $[\hat{N}, \hat{H}] = 0$

(ii) $\langle\psi|\hat{N}|\psi\rangle = N$, the number of particles in state ψ (if it has a definite number of particles)

It should be obvious by now that

$$\hat{N} = \int dk\, a_k^\dagger a_k = \int (dk)\, \alpha_k^\dagger \alpha_k$$

satisfies the above conditions.

We will see later how to generalize these statements to when we include interactions. The startegy will be to derive the form of $\hat{p}^\mu$ and $\hat{N}$ from conserved currents associated with symmetries of $\mathcal{L}$.

Time evolution We have quantized at $t = 0$. In the Heisenberg representation fields have time dependence. So consider $\hat{\phi}(x,t)$, with $\hat{\phi}(x,0)$ corresponding to the field we denoted by $\hat{\phi}(x)$ at $t = 0$ above. Note that the initial choice $t = 0$ is arbitrary since we have time translation invariance (the Lagrangian does not depend explicitly on time). Now,

$$\partial_t \hat{\phi}(x,t) = \hat{\pi}(x,t) = i[\hat{H}, \hat{\phi}(x,t)]\,.$$

The solution is well known,

$$\hat{\phi}(x,t) = e^{iHt}\hat{\phi}(x)e^{-iHt}\,.$$

To understand how this operator acts on the Fock space we cast it in terms of creation and annihilation operators. To this end we invert (2.4)

$$\begin{aligned} \alpha_k &= \omega_k \widetilde{\phi}(k) + i\widetilde{\pi}(k) \\ \alpha_{-k}^\dagger &= \omega_k \widetilde{\phi}(k) - i\widetilde{\pi}(k) \end{aligned} \qquad \Rightarrow \qquad \begin{aligned} \widetilde{\phi}(k) &= \frac{1}{2\omega_k}\left(\alpha_k + \alpha_{-k}^\dagger\right) \\ \widetilde{\pi}(k) &= -\frac{i}{2\omega_k}\left(\alpha_k - \alpha_{-k}^\dagger\right) \end{aligned}$$

Hence

$$\hat{\phi}(x) = \int (dk) \left(\alpha_k e^{ikx} + \alpha_k^\dagger e^{-ikx} \right) .$$

The time dependence is now straightforward:

$$\begin{aligned} \hat{\phi}(x,t) = e^{iHt}\hat{\phi}(x)e^{-iHt} &= \int (dk) \left(\alpha_k e^{-iE_k t + ikx} + \alpha_k^\dagger e^{iE_k t - ikx} \right) \\ &= \int (dk) \left(\alpha_k e^{-ik\cdot x} + \alpha_k^\dagger e^{ik\cdot x} \right) , \end{aligned}$$

where in the last line we have introduced $k^\mu = (E,k)$ and $x^\mu = (t,x)$ to make relativistic invariance explicit. Clearly $\hat{H}$, $\hat{p}$ and $\hat{N}$ are time independent; this is easily seen by taking $\alpha_k \to e^{-iE_k t}\alpha_k$ in the expressions for $\hat{H}$, $\hat{p}$ and $\hat{N}$). Noe the presence of positive and negative energies in $\hat{\phi}(x,t)$. But there are no “negative energy states.” Instead there are annihilation operators that subtract honestly positive energies form states, and creation operators that add it.

Note that the field $\hat{\phi}(x,t)$ satisfies the equation of motion,

$$\left(\partial_t^2 - \partial_x^2 + m^2 \right) \hat{\phi}(x,t) = 0$$

This should be the case, as expected from the commutation relations $\partial_t \hat{\pi} = i[\hat{H}, \hat{\pi}]$ and $\partial_t \hat{\phi} = i[\hat{H}, \hat{\phi}]$. But we can verify this directly from the expansion in creation and annihilation operators using

$$(\partial_t^2 - \partial_x^2) e^{-iE_k t + ikx} = -(E_k^2 - k^2) e^{-iE_k t + ikx} = -m^2 e^{-iE_k t + ikx} ,$$

or in relativistic notation,

$$\partial^2 e^{-ik\cdot x} = -k^2 e^{-ik\cdot x} = -m^2 e^{-ik\cdot x} .$$

Momentum Operator We would like the momentum operator to be defined so that $i\hat{p}$ generates translations (and is conserved). We have already defined the operator, so we check now that it does what we want:

$$\begin{aligned} [\hat{p}, \phi(x,t)] &= \int (dk')(dk) \left[k' \alpha_{k'}^\dagger \alpha_{k'}, \alpha_k e^{-iE_k t + ikx} + \alpha_k^\dagger e^{iE_k t - ikx} \right] \\ &= \int (dk) k \left(-\alpha_k e^{-iE_k t + ikx} + \alpha_k^\dagger e^{iE_k t - ikx} \right) \\ &= i\partial_x \int (dk) \left(\alpha_k e^{-iE_k t + ikx} + \alpha_k^\dagger e^{iE_k t - ikx} \right) \\ &= i\partial_x \hat{\phi}(x,t) . \end{aligned}$$

Moreover,

$$[\hat{p}, \hat{H}] = 0$$

so $\hat{p}$ is a constant in time, that is, it is conserved.

Causality While the vanishing of the equal-time commutation relation, $[\phi(x',0),\phi(x,0)] = 0$, was assumed from the start, there is no reason to suspect an analogous result for non-equal times. Let's compute,

$$\begin{aligned}[\phi(x,t),\phi(x',t')] &= \int (dk)(dk')\left[\alpha_k e^{-ik\cdot x} + \alpha_k^\dagger e^{ik\cdot x}, \alpha_{k'} e^{-ik'\cdot x'} + \alpha_{k'}^\dagger e^{ik'\cdot x'}\right] \\ &= \int (dk)\left(e^{ik\cdot(x'-x)} - e^{-ik\cdot(x'-x)}\right) \qquad (2.8)\end{aligned}$$

Notice that the right hand side is explicitly Lorentz invariant and only a function of the difference of 2-vectors, $x' - x$. We define

$$i\Delta(x'-x) = [\phi(x,t),\phi(x',t')] .$$

Using Lorentz invariance it is easy to prove that $\Delta(x) = 0$ for space-like x. Since $\Delta(x)$ is Lorentz invariant we can compute it in a boosted frame. For space-like x there is a boost that sets $t = 0$, that is, for space-like separation $x' - x$ there is a frame for which $t' = t$. The commutator vanishes at equal times, and we can then boost back to the original frame to obtain $\Delta(x) = 0$ for $x^2 < 0$. It is not difficult to verify this from the integral above by explicit calculation. One assumes $x^2 < 0$ and continues the integral of the first term in (2.8) much as was done in Fig. 1.1. The second term is continued along a contour on the lower half plane. The two terms cancel each other.

As promised causality is restored. The contribution of the positive and negative energy states cancelled each other. Only, there are no negative energy states. There are annihilation operators.

2.3 $3+1$ Dimensions

Remarkably little changes as we move on to discuss the case of 3 pace and 1 time dimensions. Now

$$L(t) = \int d^3x\, \mathcal{L} = \int d^3x \left[\tfrac{1}{2}(\partial_\mu\phi)^2 - \tfrac{1}{2}m^2\phi^2\right] ,$$

where the equality is general and the second gives the explicit case of the Lagrangian for Klein-Gordon theory. We have used $\phi = \phi(\vec{x},t) = \phi(x^\mu)$, often also denoted as $\phi(x)$, and $(\partial_\mu\phi)^2 = \eta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$ (sometimes also denoted as $(\partial\phi)^2$, we really like to compress notation). The Poisson brackets are as before, replacing $\delta^{(3)}(\vec{x}'-\vec{x})$ for $\delta(x'-x)$. This goes over directly into the quantum version. So we have equal time commutation relations

$$-i[\hat{\phi}(\vec{x},t),\hat{\pi}(\vec{x}',t)] = \delta^{(3)}(\vec{x}-\vec{x}') , \qquad [\hat{\phi}(\vec{x},t),\hat{\phi}(\vec{x}',t)] = 0 = [\hat{\pi}(\vec{x},t),\hat{\pi}(\vec{x}',t)] \qquad (2.9)$$

As before these are solved by

$$\hat{\phi}(\vec{x},0) = \int (dk)\left[\alpha_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + \alpha^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}\right]$$
$$\hat{\pi}(\vec{x},0) = -i\int (dk) E_{\vec{k}}\left[\alpha_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} - \alpha^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}\right]$$

with

$$[\alpha_{\vec{k}}, \alpha^\dagger_{\vec{k}'}] = (2\pi)^3 2E_{\vec{k}}\delta^{(3)}(\vec{k}-\vec{k}')$$
$$[\alpha_{\vec{k}}, \alpha_{\vec{k}'}] = 0 = [\alpha^\dagger_{\vec{k}}, \alpha^\dagger_{\vec{k}'}]$$

and these are interpreted as annihilation and creation operators for relativistically normalized particle states with mass m: if the vacuum state is $|0\rangle$ then

$$|\vec{k}\rangle = \alpha^\dagger_{\vec{k}}|0\rangle \qquad \text{has} \qquad \langle\vec{k}|\vec{k}'\rangle = (2\pi)^3 2E_{\vec{k}}\delta^{(3)}(\vec{k}-\vec{k}')\,.$$

After normal ordering the Hamiltonian is

$$\hat{H} = \int (dk)\, E_{\vec{k}}\, \alpha^\dagger_{\vec{k}} \alpha_{\vec{k}}\,.$$

The conserved operator

$$\hat{N} = \int (dk) \alpha^\dagger_{\vec{k}} \alpha_{\vec{k}}\,.$$

counts number of particles and

$$\hat{\vec{p}} = \int (dk)\, \vec{k}\, \alpha^\dagger_{\vec{k}} \alpha_{\vec{k}}\,.$$

are the conserved momentum operators and generate translations. As before the particles are identical and multiplarticle states satisfy Bose-Einstein statistics. In contrast to the $1+1$ case, in 3-spatial dimensions we can speak meaningfully of the spin of a particle. It must correspond to a quantum number that transforms under rotations. Our field is invariant under Lorentz transformations, $\phi(x) \to \phi'(x) = \phi(x')$, where $x' = \Lambda x$, and this is results in spinless particles. The spin-statistics connection comes out automatically: spin-0 identical particles satisfy Bose-Einstein statistics.

Time evolution is still given by

$$\begin{aligned}\hat{\phi}(x) = \hat{\phi}(\vec{x},t) &= e^{iHt}\phi(\vec{x},0)e^{-iHt}\\ &= \int (dk)\left[\alpha_{\vec{k}} e^{i\vec{k}\cdot\vec{x}-iE_{\vec{k}}t} + \alpha^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}+iE_{\vec{k}}t}\right]\\ &= \int (dk)\left[\alpha_{\vec{k}} e^{-ik\cdot x} + \alpha^\dagger_{\vec{k}} e^{ik\cdot x}\right]\end{aligned}$$

where $k^0 = E_{\vec{k}}$. The operator $\hat{\phi}(x)$ satisfies the Klein-Gordon equation,

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

which is the Euler-Lagrange equation for the Lagrangian density given above.

We will encounter later the product $\hat{\phi}(x_1)\hat{\phi}(x_2)$, and we will need its relation to the normal ordered product $:\hat{\phi}(x_1)\hat{\phi}(x_2):$. It is convenient to introduce "positive and negative frequency operators,"

$$\begin{aligned}
\hat{\phi}^{(-)}(x) &= \int (dk) e^{ik\cdot x}\alpha^\dagger_{\vec{k}}\,,\\
\hat{\phi}^{(+)}(x) &= \int (dk) e^{-ik\cdot x}\alpha_{\vec{k}}\,.
\end{aligned}$$

Then

$$\begin{aligned}
\hat{\phi}(x_1)\hat{\phi}(x_2) &= \left(\hat{\phi}^{(+)}(x_1) + \hat{\phi}^{(-)}(x_1)\right)\left(\hat{\phi}^{(+)}(x_2) + \hat{\phi}^{(-)}(x_2)\right)\\
&= \hat{\phi}^{(+)}(x_1)\hat{\phi}^{(+)}(x_2) + \hat{\phi}^{(+)}(x_1)\hat{\phi}^{(-)}(x_2) + \hat{\phi}^{(-)}(x_1)\hat{\phi}^{(+)}(x_2) + \hat{\phi}^{(-)}(x_1)\hat{\phi}^{(-)}(x_2)\\
&= \hat{\phi}^{(+)}(x_1)\hat{\phi}^{(+)}(x_2) + \hat{\phi}^{(-)}(x_2)\hat{\phi}^{(+)}(x_1) + \hat{\phi}^{(-)}(x_1)\hat{\phi}^{(+)}(x_2)\\
&\qquad + \hat{\phi}^{(-)}(x_1)\hat{\phi}^{(-)}(x_2) + [\hat{\phi}^{(+)}(x_1), \hat{\phi}^{(-)}(x_2)]\\
&= :\hat{\phi}(x_1)\hat{\phi}(x_2): + [\hat{\phi}^{(+)}(x_1), \hat{\phi}^{(-)}(x_2)]
\end{aligned}$$

Hence the difference between the product and the normal ordered product is a c-number,

$$\begin{aligned}
\Delta_+(x_2 - x_1) &\equiv [\hat{\phi}^{(+)}(x_1), \hat{\phi}^{(-)}(x_2)]\\
&= \int (dk_1)(dk_2)\, e^{ik_1\cdot x_1 - ik_2\cdot x_2}[\alpha_{\vec{k}_1}, \alpha^\dagger_{\vec{k}_2}]\\
&= \int (dk)\, e^{-ik\cdot(x_2 - x_1)}\,. \qquad (2.10)
\end{aligned}$$

That Δ_+ is only a function of the difference is the result of the explicit calculation above. You may recognize this as the integral in (1.1). Note that

$$\left(\partial^2 + m^2\right)\Delta_+(x) = 0 \qquad \text{for } x \neq 0,$$

so $\Delta_+(x)$ is a solution of the Klein-Gordon equation that does not vanish for spacelike argument.

Quantum theory is weird, of course, but QFT is even weirder. Consider this. The expectation value of $\hat{\phi}(x)$ in the vacuum state is zero at any point x,

$$\langle 0|\hat{\phi}(x)|0\rangle = 0$$

But the expectation value of the square $\hat{\phi}^2(x)$ is infinite:

$$\langle 0|\hat{\phi}^2(x)|0\rangle = \Delta_+(0) = \int (dk)\,.$$

Fluctuations of quantum fields at any point are wild, even for the simplest empty state! The problem arises from localization: we should not insist in determining the field precisely in an arbitrarily small region of space (in this case, one point). In homework you will show that the square remains finite for the field smeared over a region.