2. Canonical quantization of free scalar fields

From now on we work in units such that $\hbar = c = 1$. The free scalar field Lagrangian is $\mathcal{L} = \frac{1}{2}\partial^\mu\varphi\partial_\mu\varphi - \frac{1}{2}m^2\varphi^2$ and the Euler-Lagrange equation is the Klein-Gordon: $\partial^\mu\partial_\mu\varphi + m^2\varphi = 0$ or $(\Box + m^2)\varphi = 0$. Two solution are plane wave solutions: $\varphi(\vec{x},t) = e^{\pm i\omega t + i\vec{k}\cdot\vec{x}}$ where $\vec{k}$ is an arbitrary wave vector and $\omega = \sqrt{\vec{k}^2 + m^2}$

Therefore the general solution would be a "linear combination" of thes two solutions, but since $\vec{k}$ is a continuum parameter this linear combination is actually an integral:

$$\varphi(\vec{x},t) = \int \frac{d\vec{k}}{N(k)}\left(a(\vec{k})\, e^{-i\omega t + i\vec{k}\cdot\vec{x}} + b(\vec{k})\, e^{i\omega t + i\vec{k}\cdot\vec{x}}\right)$$

where $N(k)$ is a normalization factor and we assume suitable boundary conditions at spacial infinite in order to make the integral finite.

Since φ is real, we have conditions on the coefficients:

$$\varphi^*(\vec{x},t) = \int \frac{d\vec{k}}{N(k)} \left(a^*(\vec{k})\, e^{i\omega t - i\vec{k}\cdot\vec{x}} + b^*(\vec{k})\, e^{-i\omega t - i\vec{k}\cdot\vec{x}} \right)$$

$$= \int \frac{d\vec{k}}{N(k)} \left(a^*(\vec{k})\, e^{i\omega t - i\vec{k}\cdot\vec{x}} + b^*(-\vec{k})\, e^{-i\omega t + i\vec{k}\cdot\vec{x}} \right)$$

where in the second line we made the substitution $\vec{k} \mapsto -\vec{k}$ in the second term. Since $\varphi^*(\vec{x},t) = \varphi(\vec{x},t)$ we obtain $b^*(-\vec{k}) = a(\vec{k})$, or $a^*(-\vec{k}) = b(\vec{k})$.

Plugging back in the original solution:

$$\varphi(\vec{x},t) = \int \frac{d\vec{k}}{N(k)} \left(a(\vec{k})\, e^{-i\omega t + i\vec{k}\cdot\vec{x}} + a^*(-\vec{k})\, e^{i\omega t + i\vec{k}\cdot\vec{x}} \right)$$

Again changing $\vec{k} \mapsto -\vec{k}$ in the second integral,

$$\varphi(\vec{x},t) = \int \frac{d\vec{k}}{N(k)} \left(a(\vec{k})\, e^{-i\omega t + i\vec{k}\cdot\vec{x}} + a^*(\vec{k})\, e^{i\omega t - i\vec{k}\cdot\vec{x}} \right)$$

$$= \int \frac{d\vec{k}}{N(k)} \left(a(\vec{k})\, e^{-ikx} + a^*(\vec{k})\, e^{ikx} \right)$$

where $kx = k^\mu x_\mu = \omega t - \vec{k}\cdot\vec{x}$

(*): if we have a Lorentz transformation $x' = \Lambda x$ then $dx' = |\det\Lambda|\, dx = dx$ since $\det\Lambda = \pm 1$. But here we have a spatial integral only ($d\vec{k}$) so we don't necessarily have that the Jacobian for spatial coordinates is 1.

Finally we set up the normalization $N(k)$.

We choose $N(k) = (2\pi)^3 2\,\omega(\vec{k})$ because this makes the measure $\frac{d\vec{k}}{(2\pi)^3 2\omega}$ Lorentz invariant(*) (RS vol 2 p. 70ff; we give a proof in the appendix). So we have

$$\varphi(\vec{x},t) = \varphi(x) = \int \frac{d\vec{k}}{(2\pi)^3 2\omega} \left(a(\vec{k})\, e^{-ikx} + a^\dagger(\vec{k})\, e^{ikx} \right)$$

Now we want to invert the above equation to find $a(\vec{k})$ and $a^\dagger(\vec{k})$ in terms of φ. The equality is a Fourier like expression (indeed, it can be thought as a Fourier representation of the solution; $e^{\pm ikx}$ are the Fourier modes). Therefore we should be able to invert it. Instead of thinking of Fourier transforms, we are going to do a direct computation: first rewrite it:

$$\varphi(x) = \int \frac{d\vec{k}}{\sqrt{(2\pi)^3 2\omega}} \left(a(\vec{k}) \frac{e^{-ikx}}{\sqrt{(2\pi)^3 2\omega}} + a^\dagger(\vec{k}) \frac{e^{ikx}}{\sqrt{(2\pi)^3 2\omega}} \right)$$

$$= \int \frac{d\vec{k}}{\sqrt{(2\pi)^3 2\omega}} \left(a(\vec{k})\, f_k(x) + a^\dagger(\vec{k})\, f_k^*(x) \right)$$

where $f_k(x) = \dfrac{e^{-ikx}}{\sqrt{(2\pi)^3 2w}}$. (we follow closely Ry, p. 129)

Define $\overleftrightarrow{\partial_0}$ by $A(t)\overleftrightarrow{\partial_0}B(t) = A(t)\dfrac{\partial B(t)}{\partial t} - \dfrac{\partial A(t)}{\partial t}B(t)$

Then we check that $\{f_k\}$ forms an "orthonormal set":

$$\int d\vec{x}\, f_k^*(x)\overleftrightarrow{\partial_0} f_{k'}(x) = \int d\vec{x}\left(f_k^*(x)\frac{\partial f_{k'}(x)}{\partial t} - \frac{\partial f_k^*(x)}{\partial t} f_{k'}(x)\right)$$

$$\frac{\partial f_k}{\partial t} = \frac{1}{\sqrt{(2\pi)^3 2w}}(-iw)e^{-ikx}, \quad \frac{\partial f_k^*}{\partial t} = \frac{1}{\sqrt{(2\pi)^3 2w}}(iw)e^{ikx}, \text{ so}$$

$$= \frac{-iw}{(2\pi)^3 2w}\int d\vec{x}\left(e^{ikx}e^{-ik'x} + e^{ikx}e^{-ik'x}\right)$$

$$= -\frac{i}{(2\pi)^3}\int d\vec{x}\, e^{-i(k'-k)x}$$

Now $k = (w, \vec{k})$ and $k' = (w, \vec{k}')$, i.e, both have the same k^0 component (since we are interested in spatial components, $a(\vec{k})$ does not depend on w) so $(k'-k)x = (\vec{k}'-\vec{k})\cdot\vec{x}$, so

$$= -\frac{i}{(2\pi)^3}\int d\vec{x}\, e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}}$$, but this

is, up to the factor $-i$, a Fourier representation of the delta function (See, 41), so

$$\int d\vec{x}\, f_k^*(x)\,(i\overleftrightarrow{\partial_0})\, f_{k'}(x) = \delta(\vec{k}' - \vec{k})$$

In particular, the above calculations also imply $f_k^*(x)\,(i\overleftrightarrow{\partial_0})\, f_k^*(x) = 0$. Indeed, the first term would have an extra negative sign and we would have $-e^{ikx}e^{-ik'x} + e^{ikx}e^{-ik'x} = 0$. Going back to the field φ:

$$\varphi(x) = \int \frac{d\vec{k}}{\sqrt{(2\pi)^3 2\omega}} \left(a(\vec{k})\, f_k(x) + a^*(\vec{k})\, f_k^*(x) \right)$$

Applying $i\overleftrightarrow{\partial_0}$, multiplying by $f_{k'}^*$ and integrating over $\vec{x}$, we have that the first term gives a $\delta(\vec{k}' - \vec{k})$ which kills the integral in $\vec{k}$, and the second term vanishes, so:

$$a(\vec{k}) = \int d\vec{x}\, \sqrt{(2\pi)^3 2\omega}\; f_k^*\; i\overleftrightarrow{\partial_0}\, \varphi(x)$$

or, rewritting the original expression for f_k:

$$a(\vec{k}) = i \int d\vec{x} \; e^{ikx} \overleftrightarrow{\partial_0} \varphi(x)$$

Going back to the Lagrangian and computing the canonical momentum conjugate to φ:

$$\pi(\vec{x},t) = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}(\vec{x},t)}$$ (or, maybe it would be more precise to write $\frac{\delta \mathcal{L}}{\delta \dot{\varphi}(\vec{x},t)}$, but we stick to the abuse of notation when no confusion can arise), we find

$$\pi(\vec{x},\vec{t}) = \dot{\varphi}(\vec{x},t)$$

Finally we quantize the fields; we do this by imposing equal time commutation relations (where the fields are promoted to operators):

$$[\varphi(\vec{x},t), \varphi(\vec{x}',t)] = [\pi(\vec{x},t), \pi(\vec{x}',t)] = 0$$

$$[\varphi(\vec{x},t), \pi(\vec{x}',t)] = i\,\delta(\vec{x}-\vec{x}')$$

where t is the same for $(\vec{x},t)$ and $(\vec{x},t')$ (hence the name equal time commutation relations.

Notice that there are (at least!) two things to be clarified. The first, from a mathematical perspective, is the meaning of the commutator equal to a delta function. First, remember that in order to make QFT mathematically rigorous (when it is possible to do so) fields must be interpreted as operator valued distributions and $\varphi(x)$ would be the hypothetical operator valued function against which test functions should be averaged:

$$\varphi(f) = \int_{\mathbb{R}^4} f(x)\varphi(x)\,dx$$

but the pointwise values of $\varphi(x)$ have only formal meaning — in fact, it is possible to show that for a QFT obeying a set of natural hypothesis it is impossible to have the field as an operator valued function (RS 64, GJ 89)

The correct ~~of~~ way of thinking of the commutation is (GJ 105)

$$[\varphi(f), \pi(g)]\psi = \langle f, g\rangle \psi$$

where $\langle , \rangle$ is the L^2 inner product of f and g and ψ is any element in the domain of $\varphi(f)$ and $\pi(g)$ (for more details see GJ 105)

To see how the expression $[\ ] = \delta$ could ~~be~~ formally lead to the meaningful expression above, suppose the averaging procedure referred above were valid, then:

$$[\varphi(f), \pi(g)] = \left[\int \varphi(x) f(x)\, dx, \int \pi(x') g(x')\, dx'\right] =$$

$$= \iint \underbrace{[\varphi(x), \pi(x')]}_{= \delta(x-x')} f(x) g(x')\, dx\, dx' = \iint \delta(x-x') f(x) g(x')\, dx\, dx'$$

$$= \int f(x) g(x)\, dx = \langle f, g\rangle$$

The second issue about the equal time commutation relations is the meaning of the word "equal time". In special relativity the notion of equal time is observer dependent, so how do we want to have a quantum theory compatible with special relativity using "equal time" commutation relations? The answer is the following. If two events happen at equal time in one frame then they are space-like separated. In another frame they will no longer correspond to equal time, but they will still be space-like separated. In another words, if two events $(\vec{x}, t)$ and $(\vec{x}', t')$ are space-like separated, then there is a frame for which $t = t'$ (same time), but in this frame $\vec{x} \neq \vec{x}'$ (because the events are space-like separated) and so the commutator reads:

$$[\varphi(\vec{x}, t), \pi(\vec{x}', t)] = \delta(\vec{x}' - \vec{x}) = 0$$

So, all we are saying is that operators at space-like separated points commute ~~space~~ — a very relativistic notion, indeed! (since space-like separated points can not exchange any information).

Of course, this analysis does not hold if $t = t'$ and $\vec{x} = \vec{x}'$; but in this case φ and π are operators at the same space-time point — and so they can not commute.

All this said, let us return to the canonical commutation relations. Since now we promoted the fields to operators, the coefficients $a(\vec{k})$ and $a^{+}(\vec{k})$ become operators also (with a^{*} becoming the adjoint a^{+}). Recall that

$$a(\vec{k}) = \int d\vec{x}\, \sqrt{(2\pi)^3 2\omega}\, f_k^{*}(x)\, i\overleftrightarrow{\partial_0}\, \varphi(x)$$

the conjugate reads

$$a^{+}(\vec{k}) = \left(a^{*}(\vec{k})\right) = \int d\vec{x}\, \sqrt{(2\pi)^3 2\omega}\, \varphi(x)\, i\overleftrightarrow{\partial_0}\, f_k(x)$$

(take conjugate of $a(\vec{k})$ and use $A\overleftrightarrow{\partial_0}B = -B\overleftrightarrow{\partial_0}A$)

So we have (recall that $\omega = \omega(\vec{k})$)

$$[a(\vec{k}), a^\dagger(\vec{k}')] = \int d\vec{x}\, d\vec{x}'\, (2\pi)^3 \sqrt{4\omega(\vec{k})\,\omega(\vec{k}')}\, \Big[f_k^*(x)\, i\overleftrightarrow{\partial_0}\, \varphi(x),\ \varphi(x')\, i\overleftrightarrow{\partial_0}\, f_{k'}(x') \Big]$$

$$= \int d\vec{x}\, d\vec{x}'\, (2\pi)^3 \sqrt{4\omega(\vec{k})\,\omega(\vec{k}')}\, \Big[-i\left(\partial_0 f_k^*(x)\right)\varphi(x) + i f_k^*(x)\, \overbrace{\partial_0 \varphi(x)}^{\pi(x) \,=}\ ,$$

$$- i \underbrace{\left(\partial_0 \varphi(x')\right)}_{=\pi(x')} f_{k'}(x') + i\, \varphi(x')\, \partial_0 f_{k'}(x') \Big] ,$$ keeping only non-zero commutators

$$= \int d\vec{x}\, d\vec{x}'\, (2\pi)^3 \sqrt{4\omega(\vec{k})\,\omega(\vec{k}')} \Big(-\left(\partial_0 f_k^*(x)\right) f_{k'}(x')\, [\varphi(x), \pi(x')]$$

$$+ f_k^*(x) \left(\partial_0 f_{k'}(x')\right) [\varphi(x'), \pi(x)] \Big)$$

$$= \int d\vec{x}\, d\vec{x}'\, (2\pi)^3 \sqrt{4\omega(\vec{k})\,\omega(\vec{k}')}\, \left(f_k^*(x)\, \overleftrightarrow{\partial_0}\, f_{k'}(x') \right) \underbrace{[\varphi(x), \pi(x')]}_{= i\delta(\vec{x}-\vec{x}')}$$

$$= \int d\vec{x}\, (2\pi)^3 \sqrt{4\omega(\vec{k})\,\omega(\vec{k}')}\, f_k^*(x) \left(i\overleftrightarrow{\partial_0}\right) f_{k'}(x)$$

Again, $\int d\vec{x}\, f_k^*(x) \left(i\overleftrightarrow{\partial_0}\right) f_{k'}(x) = \delta(\vec{k}-\vec{k}')$ (see p. 15 and 16) so

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

Similarly we obtain $[a(\vec{k}), a(\vec{k}')] = [a^\dagger(\vec{k}), a^\dagger(\vec{k}')] = 0$
These three equalities tells us that the a's satisfy an oscillator algebra (with the kronicker delta replaced by the Dirac delta now that we have infinite number of degrees of freedom). Therefore they should be interpreted as creation and annihilation operators ($a^\dagger(\vec{k})$ is creation and $a(\vec{k})$ is annihilation).

The procedure which concludes from the commutation relation that $a^\dagger$ and a are creation and annihilation operators is a standard construction for the harmonic oscillator so we ommit it here (see Ry 129ff or St 38 ff. or the appendix)

In particular, a state of n particles with momenta $k_1, \dots, k_n$ and mass m is given by

$|k_1 \cdots k_n\rangle = a^\dagger(\vec{k}_1) \cdots a^\dagger(\vec{k}_n)|0\rangle$ where $|0\rangle$ is the vacuum.