1. The Free Scalar Field

1. THE FREE SCALAR FIELD

To begin with, we will approach quantum field theory by starting with a (relativistic) classical theory, and then performing canonical quantization. (Canonical quantization is a procedure for formulating a quantum theory with a given classical limit.) This may be a perverse choice of a place to begin if our real interest is in particles, but we will be able to justify it in retrospect.

So, to get started, we need to specify a relativistically invariant (frame-independent) classical dynamics for a field or set of fields, and we'll consider, at first, the simplest case, that of a single scalar field.

Scalar refers to the transformation properties of the field under a Lorentz transformation.

Lorentz Group

... is the group of linear transformations that preserve the spacetime interval $t^2 - \vec{x}^2$

We'll denote $x^\mu = (t, \vec{x})$, $\mu = 0, 1, 2, 3$

$$x^2 = (x^0)^2 - (x^1)^2 - (x^2)^2 - (x^3)^2$$

$$= x^\mu \eta_{\mu\nu} x^\nu = x^\mu x_\mu$$

(Note: units with $c = 1$)

where $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$

Lorentz transformation:

$$x^\mu \to \Lambda^\mu{}_\nu x^\nu$$

$$x^2 \to \eta_{\mu\nu} \Lambda^\mu{}_\lambda \Lambda^\nu{}_\rho x^\lambda x^\rho = x^2 \text{ (for any } x\text{)}$$

$$\Rightarrow \eta_{\mu\nu} \Lambda^\mu{}_\lambda \Lambda^\nu{}_\rho = \eta_{\lambda\rho} \quad \text{or} \quad \Lambda^T \eta \Lambda = \eta$$

(in matrix notation)

This group is $O(3,1)$. (But by "Lorentz group" I'll generally mean its connected component $SO(3,1)$.)

A field ϕ is a (real) function of spacetime $\phi(x)$. Scalar field means, under a Lorentz trans. Λ

$$\phi(x) \longrightarrow \phi(x') \quad \text{where } x' = \Lambda x$$

is a new coord system

-- ϕ is a tensor of zero rank

The classical dynamics of ϕ is Lorentz-invariant (independent of frame) if the eqn of motion is unchanged when x is replaced by x' (or if Action is left invariant by a Lorentz transformation)

The action $S[\phi]$ is a functional of the field $\phi(t,\vec{x})$. As in particle mechanics, we demand that S involves no higher time derivatives of ϕ than the first derivative; this is so that ϕ will have a well-formulated "initial value problem": when $\phi(t_0,\vec{x})$ and its first time derivative $\dot{\phi}(t_0,\vec{x})$ are specified at an initial time t_0 (or some initial spacelike 3-surface), they are determined by the classical eqns at all subsequent times. In a relativistic theory, higher spatial derivatives than the first will also be forbidden.

If we want a causal theory, action should be local in spacetime; there should be no terms that couple ϕ's (or derivatives) at different spacetime points.

With these conditions imposed, the action has the form:

$$S = \int d^4x \, \mathcal{L}(\partial_\mu \phi(x), \phi(x))$$

I've also demanded translation invariance -- homogeneity of space and time, so that $\mathcal{L}$ has no explicit dependence on x.

(Here $\partial_\mu \phi$ denotes $\frac{\partial}{\partial x^\mu}\phi$ -- note downstairs index)

Now we'll consider an important special case, the free scalar field theory. The free theory has a linear eqn of motion, and hence is exactly solvable, both classically and quantum mechanically. (compare the harmonic oscillator in mechanics.) The action is quadratic in ϕ.

What are the possible quadratic terms in $\mathcal{L}$? Remember that we want S to be Lorentz-invariant. Since the measure

$$d^4x = dt\, d^3x$$

is Lorentz-invariant, $\mathcal{L}$ must be Lorentz-invariant (or change by a total derivative under a Lorentz trans) the only possible terms are --

$$\partial^\mu \phi \, \partial_\mu \phi \quad \text{and} \quad \phi^2$$ (Can "shift" away a linear term in ϕ)

(We exclude $\phi \partial_\mu \phi$ because it is not Lorentz inv.,
$\int dy\, \phi(y) f(y-x) \phi(x)$ because it is not local
ϕ^3 because it is not quadratic
etc.)

So the most general possible action for the free scalar field theory is

$$S = \int d^4x \left[\tfrac{1}{2} \partial_\mu \phi(x) \partial^\mu \phi(x) - \tfrac{1}{2} m^2 \phi(x)^2 \right]$$

($m^2 > 0$, for energy bounded below)

(If the $(\partial\phi)^2$ term had some other coefficient, we could rescale ϕ to absorb it, as long as it were positive) Thus, the free scalar field theory has just one arbitrary parameter, m^2. It obviously has the dimensions of $(\text{length})^{-2}$. In the units we'll usually use, with $\hbar = c = 1$, this is the same as $(\text{mass})^2$

We've now formulated a classical field theory, which we wish to quantize. How do we proceed? We should think of $\phi(t, \vec{x})$ as a set of dynamical variables indexed by $\vec{x}$, and proceed with canonical quantization.

Review of Canonical Quantization:

Consider a classical theory with N degrees of freedom,

$$S = \int_{t_1}^{t_2} dt \; L(q^a, \dot{q}^a), \quad a = 1, 2, \ldots, N$$

the classical eqn of motion is found by extremizing S (with q^a fixed at endpoints)

$$\delta S = 0 = \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial \dot q^a} \delta \dot q^a + \frac{\partial L}{\partial q^a} \delta q^a \right]$$

$$= \int dt \; \delta q^a \left[-\frac{d}{dt} \frac{\partial L}{\partial \dot q^a} + \frac{\partial L}{\partial q^a} \right] \qquad \text{(integrate by parts)}$$

$$\Rightarrow \quad 0 = -\frac{d}{dt} \frac{\partial L}{\partial \dot q^a} + \frac{\partial L}{\partial q^a} \, , \quad a = 1, \ldots, N$$

(Euler-Lagrange Eqn)

To obtain the canonical formalism, eliminate the $\dot q^a$ in favor of p_a (possible if no. of independent $\dot q^a$ and p_a is the same)

$$H(q^a, p_a) = \left[p_a \dot q_a - L(q_a, \dot q_a) \right] \Big|_{p_a = \frac{\partial L}{\partial \dot q^a}}$$

Then

$$dH = \dot q_a \, dp_a - \frac{\partial L}{\partial q_a} dq_a$$

or

$$\dot q_a = \frac{\partial H}{\partial p_a} , \quad \underbrace{\dot p_a = \frac{\partial L}{\partial q_a}}_{\text{E-L eqn}} = -\frac{\partial H}{\partial q^a} \qquad \text{(Hamiltonian Eqns.)}$$

(if p_a's and q^a's are independent)

To quantize, we elevate p's and q's to the status of operators in a Hilbert space, obeying "canonical commutation relations," which are just canonical Poisson Brackets, reinterpretted as operator commutators, with factor of $i\hbar$ inserted. We'll use the Heisenberg picture, in which operators are time dependent, so canonical commutation relations are <u>equal time</u> commutation relations:

$$[q^a(t), q^b(t)] = 0 = [p^a(t), p^b(t)]$$
$$[q^a(t), p^b(t)] = i\delta^{ab}$$
(units: $\hbar = 1$)

Time evolution is governed by the operator $H(p,q)$ -- (possible ordering ambiguity) -- according to

$$\mathcal{O}(t) = e^{iHt}\mathcal{O}(0)e^{-iHt}$$

or $$\frac{d\mathcal{O}}{dt} = -i[\mathcal{O}, H]$$ (if $\mathcal{O}$ has no <u>explicit</u> time dependence)

Since the canonical commutation relations can be "represented" by $q^a = i\frac{\partial}{\partial p^a}$ or $p^a = -i\frac{\partial}{\partial q^a}$,

we have
$$\dot{q}^a = -i[q^a, H] = \partial H/\partial p^a$$
$$\dot{p}^a = -i[p^a, H] = -\partial H/\partial q^a$$

Thus, the canonical equations of motion are satisfied as operator equations. In particular, they are satisfied in expectation value, so the classical limit of this quantum system is the classical system we began with. (Correspondence principle.)

<u>Generalization to Field Theory</u>

The action of a scalar field theory is

$$S = \int d^4x \; \mathcal{L}(\phi, \partial^\mu\phi)$$

We obtain classical eqns of motion (field eqns) by extremizing S, with ϕ held fixed on "boundary" of spacetime:

$$\delta S = \int d^4x \left[\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} \partial_\mu \delta\phi + \frac{\partial \mathcal{L}}{\partial \phi} \delta\phi \right]$$

$$= \int d^4x \; \delta\phi \left[-\partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} + \frac{\partial \mathcal{L}}{\partial \phi} \right]$$ (integrating by parts)

$$\Longrightarrow \quad \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} - \frac{\partial \mathcal{L}}{\partial \phi} = 0$$

In the case of the free scalar field,

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

the equation of motion is

$$\partial_\mu \partial^\mu \phi + m^2 \phi = 0.$$ (Klein-Gordon Eqn.)

This is a linear equation that can be easily solved by Fourier transforming:

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

then $\quad \frac{\partial^2}{\partial t^2} \tilde{\phi}(t, \vec{k}) = -(\vec{k}^2 + m^2)\, \tilde{\phi}(t, \vec{k})$

This has the general solution:

$$\tilde{\phi}(t, \vec{k}) = A(\vec{k}) e^{-i\omega_k t} + B(\vec{k}) e^{i\omega_k t},$$

where $\quad \omega_k = +\sqrt{\vec{k}^2 + m^2}.$

Furthermore, $\phi(t, \vec{x})$ is real, so $\tilde{\phi}(\vec{k}) = \tilde{\phi}(-\vec{k})^*$. Thus

$$\tilde{\phi}(t, \vec{k}) = A(\vec{k}) e^{-i\omega_k t} + A(-\vec{k})^* e^{i\omega_k t}$$

So the general solution is:

$$\phi(t,\vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}}\Big[A(\vec{k})e^{-i\omega_k t}e^{i\vec{k}\cdot\vec{x}} + A(\vec{k})^* e^{i\omega_k t}e^{-i\vec{k}\cdot\vec{x}}\Big]$$

(changing variables $\vec{k}\to-\vec{k}$ in the second term).
We'll sometimes write this as

$$\phi(x) = \int\frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\Big[a(\vec{k})e^{-ik\cdot x} + a(\vec{k})^* e^{ik\cdot x}\Big],$$

with the understanding $k_0 = \omega_k$ in the exponent

$$k\cdot x = k^0x^0 - \vec{k}\cdot\vec{x}.$$

I have also, by convention, renormalized the coefficients $A(\vec{k}) = a(\vec{k})/\sqrt{2\omega_k}$. The reason for this peculiar convention will be clear later. (Note: both + and − frequencies.)

Proceeding with our review of the canonical formalism, we construct a Hamiltonian by

$$H(\pi,\phi) = \underset{\dot\phi}{\mathrm{Ext}}\int d^3x\,[\pi\dot\phi - \mathcal{L}(\phi,\partial_\mu\phi)]$$

The canonical momentum $\pi(x)$ is a field, the functional derivative of L

$$\pi(x) = \frac{\delta L}{\delta\dot\phi(x)} = \frac{\partial\mathcal{L}}{\partial\dot\phi(x)}$$

-- or the partial derivative of the Lagrange density

All of Hamiltonian mechanics generalizes in this way, with partial derivatives $\frac{\partial}{\partial q}, \frac{\partial}{\partial p}$ replaced by functional derivatives $\frac{\delta}{\delta\phi(x)}, \frac{\delta}{\delta\pi(x)}$

In the free scalar field theory.

$$H = \int d^3x \left[\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\vec{\nabla}\phi)^2 + \tfrac{1}{2}m^2\phi^2 \right]$$

(We choose $m^2 > 0$ so that H is bounded from below -- $\phi = 0$ is a stable solution.)

Quantization: equal time commutation relations become

$$[\phi(\vec{x},t), \phi(\vec{y},t)] = 0$$
$$[\pi(\vec{x},t), \pi(\vec{y},t)] = 0$$
$$[\phi(\vec{x},t), \pi(\vec{y},t)] = i\,\delta^3(\vec{x}-\vec{y})$$

Comments:

- Note the continuum normalization; the Dirac δ-function in commutator indicates that the fields are singular distributions -- this will be a source of infinities. To be mathematically well-defined, fields should be "smeared". For example, smearing in space at fixed time:

$$\phi(f,t) = \int d^3x \; \phi(\vec{x},t) f(\vec{x})$$

$$[\phi(f,t), \pi(g,t)] = i\int d^3x \, f(\vec{x})\, g(\vec{x})$$

- Treating fields as Heisenberg operators is natural. The fields depend on $\vec{x}$, so they ought to be permitted to depend on t as well.

- However, the quantization procedure obviously spoils Lorentz invariance, it is frame-dependent; "equal time" is a relative concept. Further, the Hamiltonian H is one component of a 4-vector, but is given a special status as the generator of the evolution of the system. After the quantization procedure is carried out, we are obligated to check that the quantum theory does not really depend on the choice of frame that we made.

- Note that the canonical quantization procedure may be trivially generalized to a theory involving any number of scalar fields.

Now, let's construct the Hamiltonian of the quantum theory. Since

$$\pi(x) = \dot{\phi}(x),$$

we have

$$H = \int d^3x \left[\tfrac{1}{2}\dot{\phi}^2 + \tfrac{1}{2}(\vec{\nabla}\phi)^2 + \tfrac{1}{2}m^2\phi^2 \right]$$

It is convenient to make a change of variable: Since

$$\phi(x) = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \left[a(\vec{k})e^{-ik\cdot x} + a(\vec{k})^* e^{ik\cdot x} \right]$$

solves the classical equation of motion, we may expect that $a(\vec{k})$ is a time-independent operator (in the Heisenberg representation of the quantum theory). Substituting gives (assuming $\dot{a} = 0$)

$$H = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \int \frac{d^3k'}{(2\pi)^{3/2}\sqrt{2\omega_{k'}}} \int d^3x$$

$$\Big[a(\vec{k})a(\vec{k}')(-\omega_k\omega_{k'} - \vec{k}\cdot\vec{k}' + m^2)e^{i(k+k')\cdot x}$$
$$a(\vec{k})a(\vec{k}')^+(\omega_k\omega_{k'} + \vec{k}\cdot\vec{k}' + m^2)e^{-i(k-k')\cdot x}$$
$$+ a(\vec{k})^+a(\vec{k}')(\omega_{k'}\omega_k + \vec{k}\cdot\vec{k}' + m^2)e^{i(k-k')\cdot x}$$
$$+ a(\vec{k})^+a(\vec{k}')^+(-\omega_k\omega_{k'} - \vec{k}\cdot\vec{k}' + m^2)e^{i(k+k')\cdot x}\Big]$$

Now x integral gives δ function, and one k integral is trivial, so we obtain

$$H = \int d^3k \qquad \tfrac{1}{2}\omega_k\left[a(\vec{k})a(\vec{k})^+ + a(\vec{k})^+a(\vec{k})\right]$$

(Note that we've been careful about operator ordering) We've expressed H in terms of a and a^+. Now we need to know commutation relations for these operators, which can be obtained from canonical relations. We have

$$a(\vec{k}) = i\int \frac{d^3x}{(2\pi)^{3/2}\sqrt{2\omega_k}} e^{ik\cdot x}(\dot{\phi}(x) - i\omega_k\phi(x))$$

$$a(\vec{k})^+ = i\int \frac{d^3x}{(2\pi)^{3/2}\sqrt{2\omega_k}} e^{-ik\cdot x}(-\dot{\phi}(x) - i\omega_k\phi(x))$$

Since a and a^+ are time-independent, we may choose times to be equal in evaluating --

$$[a(\vec{k}), a(\vec{k}')] = -\int \frac{d^3x}{(2\pi)^{3/2}\sqrt{2\omega_k}} e^{ik\cdot x} \int \frac{d^3x'}{(2\pi)^{3/2}\sqrt{2\omega_{k'}}} e^{-ik'\cdot x'}$$

$$\left[-i\omega_{k'}(-i)\delta^3(\vec{x}'-\vec{x}) - i\omega_k(i)\delta^3(\vec{x}-\vec{x}') \right]$$

$$= \int \frac{d^3x}{(2\pi)^3} \frac{1}{\sqrt{4\omega_k\omega_{k'}}} e^{i(\omega_k-\omega_{k'})t}(\omega_{k'}-\omega_k)e^{i(\vec{k}'-\vec{k})}$$

$$= \tfrac{1}{2} e^{i(\omega_k-\omega_{k'})t}\left(\sqrt{\frac{\omega_{k'}}{\omega_k}} - \sqrt{\frac{\omega_k}{\omega_{k'}}}\right)\delta^3(\vec{k}'-\vec{k})$$

$$= 0$$

Similarly,

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

But --

$$[a(\vec{k}), a(\vec{k}')^+] = \tfrac{1}{2} e^{i(\omega_k-\omega_{k'})t}\left(\sqrt{\frac{\omega_{k'}}{\omega_k}} + \sqrt{\frac{\omega_k}{\omega_{k'}}}\right)\delta^3(\;)$$

$$= \delta^3(\vec{k}-\vec{k}')$$

Thus, the $a(\vec{k})$'s are just like the destruction operators for a set of uncoupled harmonic oscillators, but with continuum normalization. The free field theory is a set of oscillators, each oscillator corresponding to a mode of vibration of the field ϕ.

Returning to the expression for the Hamiltonian, we have

$$H = \int d^3k \left[\omega_k a(\vec{k})^+ a(\vec{k}) + \tfrac{1}{2}\omega_k \delta(0) \right]$$

So H contains an *infinite* additive constant. How do we interpret this constant?

-- the ground state of all the oscillators (the vacuum) is the state such that

$$a(\vec{k})|0\rangle = 0 \quad , \text{ for all } \vec{k}$$

This is an eigenstate of H, with

$$H|0\rangle = \left(\int d^3k \;\; \delta(0)\, \tfrac{1}{2}\omega_k\right)|0\rangle = E_0|0\rangle$$

-- the infinite constant is the *vacuum energy*.

Not just the energy, but the energy *density* is infinite. Writing $\delta(0) = \int \frac{d^3x}{(2\pi)^3}$, we have

$$E_0 = \int d^3x \int \frac{d^3k}{(2\pi)^3}\, \tfrac{1}{2}\omega_k = \sum_{\vec{k}} \tfrac{1}{2}\omega_k$$

Now $\dfrac{d^3k}{(2\pi)^3}$ is the density of states

-- this is just the sum of the zero point energies of all the oscillators

This is the first of various infinities that arise in quantum field theory. How should we deal with it?

- We can just subtract it away! It is just an additive constant in the energy, and where we define the zero of energy is arbitrary

- We can take the attitude that the infinity arises as a consequence of an ordering ambiguity. Classically, we have

$$H = \int d^3k \ \tfrac{1}{2}\omega_k \left[a(\vec{k})^\dagger a(\vec{k}) + a(\vec{k})^\dagger a(\vec{k}) \right],$$

but classically a and $a^\dagger$ commute, so we can change the ordering before promoting a and $a^\dagger$ to operators in Hilbert space. One way of resolving the ordering ambiguity is to adopt the convention that a will always be on the right of $a^\dagger$ (normal ordering)

$$:H: = \int d^3x : \tfrac{1}{2}\left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2 \right]:$$

$$= \int d^3k \ \omega_k \, a(\vec{k})^\dagger a(\vec{k})$$

- This infinity appears to be fairly innocuous, but it is, in fact, the deepest of all infinities in field theory, in a certain sense. The one case in which we are not free to adjust the zero of energy is in a theory of gravity. In the real world, why doesn't the zero point energy of all oscillators gravitate, curling spacetime into a tiny ball -- the "cosmological constant" problem.

One aspect of the above discussion may be confusing; we assumed $a(\vec{k})$ to be time independent, but Ken found that a does not commute with H. What is going on?

To understand, suppose we have an oscillator with one degree of freedom

$$H = \omega a^\dagger a \qquad [a, a^\dagger] = 1$$

$$\frac{da}{dt} = -i[a, H] = -i\omega a$$

Now define $a' = e^{i\omega t} a$

then $$\frac{da'}{dt} = -i[a', H] + \frac{\partial a'}{\partial t} = -i\omega a' + i\omega a' = 0$$

So a' is time independent, because of its explicit time-dependence. Our $a(\vec{k})$ is like a', as we can readily from expression on page 1.11.

Another way to derive the above results is to begin with the Hamiltonian

$$H = \int d^3x \ \tfrac{1}{2}\left[\pi(x)^2 + (\vec{\nabla}\phi(x))^2 + m^2\phi(x)^2\right]$$

and then diagonalize this quadratic form by going to momentum space -- expanding in "normal modes":

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

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

Thus

$$H = \int d^3k \left[\tfrac{1}{2}\tilde{\pi}(\vec{k}, t)\tilde{\pi}(-\vec{k}, t) + \tfrac{1}{2}(k^2 + m^2)\tilde{\phi}(\vec{k}, t)\tilde{\phi}(-\vec{k}, t)\right]$$

and $$[\phi, \phi] = [\pi, \pi] = 0, \quad [\phi(\vec{x}, t), \pi(\vec{x}', t)] = i\delta(\vec{x} - \vec{x}')$$

$$\Rightarrow [\tilde{\phi}, \tilde{\phi}] = [\tilde{\pi}, \tilde{\pi}] = 0, \quad [\tilde{\phi}(\vec{k}, t), \tilde{\pi}(\vec{k}', t)] = i\delta(\vec{k} + \vec{k}')$$

This is evidently a sum of uncoupled oscillators. If we define

$$a(\vec{k},t) = i \left[\frac{1}{\sqrt{2\omega_k}} \tilde{\pi}(\vec{k},t) - i\sqrt{\frac{\omega_k}{2}}\, \tilde{\phi}(\vec{k},t) \right]$$

$$a^{+}(\vec{k},t) = i \left[\frac{1}{\sqrt{2\omega_k}} -\tilde{\pi}(-\vec{k},t) - i\sqrt{\frac{\omega_k}{2}}\, \tilde{\phi}(-\vec{k},t) \right]$$

π, ϕ real, so $\quad \pi(-\vec{k},t) = \pi(\vec{k},t)^{+}$

$\phi(-\vec{k},t) = \phi(\vec{k},t)^{+}$

then

$$\omega_k\left[a(\vec{k},t)\,a(\vec{k},t)^{+} + a(\vec{k},t)^{+}a(\vec{k},t)\right]$$

$$= \pi(\vec{k},t)\,\pi(-\vec{k},t) + \omega_k^2\, \phi(\vec{k},t)\,\phi(-\vec{k},t)$$

and $\quad [a,a] = [a^{+},a^{+}] = 0$

$$[a(\vec{k},t),\, a^{+}(\vec{k}',t)] = \delta(\vec{k}-\vec{k}')$$

Now

$$\dot{a}(\vec{k},t) = -i[a(\vec{k},t), H]$$

$$= -i\omega_k\, a(\vec{k},t)$$

$\Rightarrow$

$$a(\vec{k},t) = e^{-i\omega_k t}\, a(\vec{k},0)$$

we may write

$$b(\vec{k}) = e^{i\omega_k t}\, a(\vec{k},t)$$ -- A time-independent operator

Now $\tilde{\phi}(\vec{k},t) = \frac{1}{\sqrt{2\omega_k}}\left[a(\vec{k},t) + a(-\vec{k},t)^+\right]$

$$= \frac{1}{\sqrt{2\omega_k}}\left[e^{-i\omega_k t}\, b(\vec{k}) + e^{i\omega_k t}\, b(-\vec{k})^+\right]$$

and

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

$$= \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\left[e^{-ik\cdot x} a(\vec{k}) + e^{ik\cdot x} a(\vec{k})^+\right.$$

-- We've replaced b by a, changed $\vec{k} \to -\vec{k}$ in second term, and written

$k\cdot x = k^0 t - \vec{k}\cdot\vec{x}$, where $k^0 = \omega_k$

Free Particles (Fock Space)

Since the Hamiltonian of the free scalar field

$$H = \int d^3k \; \omega_k \quad a(\vec{k})^+ a(\vec{k})$$

is just the sum of uncoupled oscillators, it is trivial to diagonalize it.

For this purpose, it may be conceptually easier to imagine that system is in a cubic box of size L, with field ϕ obeying periodic boundary conditions: then momenta take discrete values

$$\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$$

-- that is the mode expansion of the field ϕ has the form

$$\phi(x) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} \frac{1}{\sqrt{2\omega_k}} \left[e^{-ik\cdot x} a_{\vec{k}} + e^{ik\cdot x} a_{\vec{k}}^+ \right]$$

$(V = L^3)$ then, if a's have the discrete normalization

$$[a_{\vec{k}}, a^+_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$$

ϕ and $\dot{\phi}$ obey the canonical commutation relations, since --

$$\delta^3(\vec{x}-\vec{x}') = \frac{1}{V} \sum e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')}$$

In this representation the Hamiltonian is

$$H = \sum_{\vec{k}} \omega_k \, a_{\vec{k}}^+ a_{\vec{k}}$$

The Hilbert space on which H acts is evidently an ∞ direct product of oscillator spaces, and the ground state is the product of all oscillator ground states

$$|0\rangle = \prod_{\vec{k}} |0\rangle_{\vec{k}} \quad \text{where} \quad a_{\vec{k}}|0\rangle_{\vec{k}} = 0$$

In an arbitrary eigenstate of H, each oscillator may be excited:

$$|n\rangle_{\vec{k}} = \frac{1}{\sqrt{n!}} (a^{+}_{\vec{k}})^{n} |0\rangle_{\vec{k}}$$

The $\frac{1}{\sqrt{n!}}$ ensures that these states are properly normalized (if $|0\rangle$ is):

$${}_{\vec{k}}\langle n'|n\rangle_{\vec{k}} = \delta_{n,n'}$$

Thus, an arbitrary eigenstate can be specified by a function $n_{\vec{k}}$ that takes values in nonnegative integers

$$|n_{\vec{k}}\rangle = \prod_{\vec{k}} \frac{(a^{+}_{\vec{k}})^{n_{\vec{k}}}}{\sqrt{n_{\vec{k}}!}} |0\rangle_{\vec{k}}$$

The energy of this state is

$$H|n_{\vec{k}}\rangle = \sum_{\vec{k}} n_{\vec{k}} \omega_k$$

Since the excitations of each oscillator are uniformly spaced these states have an obvious interpretation: the oscillator excitations are noninteracting particles -- Quanta of the field. Thus free particle

Hilbert space is called a Fock space

We'll typically be interested in states with finite no. of particles, $\sum n_{\vec{k}} < \infty$, and we'll usually find it convenient to denote such a state

$$|\vec{k}_1, \ldots, \vec{k}_n\rangle = a(\vec{k}_1)^\dagger \ldots a(\vec{k}_n)^\dagger |0\rangle$$

(with appropriate factors of $\sqrt{n!}^{-1}$ understood, if momenta coincide) Returning to the continuum normalization, one particle states have the normalization

$$\langle \vec{k}' | \vec{k}\rangle = \langle 0| a(\vec{k}')\, a(\vec{k})^\dagger |0\rangle = \delta^3(\vec{k}'-\vec{k})$$

Furthermore, many particle states have the property of obeying "what is known as Bose statistics" -- they are invariant under interchanges of momenta, because $a^\dagger$'s commute. E.g.

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

is same as $|\vec{k}_2, \vec{k}_1\rangle$. The normalization of these states is

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

$$= \delta^3(\vec{k}_1'-\vec{k}_1)\,\delta^3(\vec{k}_2'-\vec{k}_2) + \delta^3(\vec{k}_1'-\vec{k}_2)\,\delta^3(\vec{k}_2'-\vec{k}_1)$$

-- consistent with Bose symmetry

(Technical Point: the Fock space is actually a small (separable) subspace of the full (nonseparable) oscillator Hilbert space, but all observables that interest us can be defined in Fock space.)

Remarks:

- We noted earlier that the canonical quantization procedure destroys covariance, but we now see that the result of carrying out this procedure has a covariant description. Each particle of momentum $\vec{k}$ has energy

$$E = \omega_k \quad \text{or} \quad E^2 - \vec{k}^2 = m^2$$

-- changing the frame boosts the momentum, but this is a Lorentz invariant relation. We also see that the free parameter m can be interpreted as mass of the free particle

- The one particle states $|\vec{k}\rangle$ are plane wave states, with continuum normalization. We can construct normalizable states as wave packets (just as in particle mechanics.) To see that states $|\vec{k}\rangle$ are not localized in space, we introduce a translation operator $\exp[i\vec{P}\cdot\vec{x}]$ such that

$$e^{i\vec{P}\cdot\vec{x}'}\phi(\vec{x},t)e^{-i\vec{P}\cdot\vec{x}'} = \phi(\vec{x}+\vec{x}',t)$$

then

$$a(\vec{k}) = i\int \frac{d^3x}{(2\pi)^{3/2}\sqrt{2\omega_k}} e^{ik\cdot x}\left[\dot\phi(\vec{x},t) - i\omega_k\phi(\vec{x},t)\right]$$

transforms as

$$e^{i\vec{P}\cdot\vec{x}'}a(\vec{k})e^{-i\vec{P}\cdot\vec{x}'} = e^{-i\vec{k}\cdot\vec{x}'}a(\vec{k})$$

(opposite sign for $a^\dagger$)

Now, if the vacuum is translation invariant (it must be, by relativity, if it has zero energy $\Rightarrow$ temporal translation invariance), then

$$e^{i\vec{P}\cdot\vec{x}}|\vec{k}\rangle = e^{i\vec{k}\cdot\vec{x}}|\vec{k}\rangle$$

So $|\vec{k}\rangle$ is a plane-wave state, but

$$|f\rangle = \int d^3k\, f(\vec{k})\, |\vec{k}\rangle \quad \text{has norm}$$

$$\langle f|f\rangle = \int d^3k\, |f(\vec{k})|^2$$ -- it is a normalizable plane wave state if f is square integrable

- We noted earlier that ϕ has the decomposition

$$\phi = \phi^- + \phi^+$$

into negative frequency and positive frequency parts. We now understand better the physical interpretation of this decomposition -- ϕ^- destroys particles, ϕ^+ creates particles

Representation of Lorentz Group

We have constructed a relativistic quantum theory. Thus we expect the Fock space, our Hilbert space, to provide a representation of the Lorentz group. That is, changing frame is equivalent to changing basis in Hilbert space in terms of which we expand states

$$|\text{state}\rangle \to U(\Lambda)\,|\text{state}\rangle$$

And if we change frame twice, consistency demands

$$U(\Lambda_1)\,U(\Lambda_2)\,|\text{state}\rangle = U(\Lambda_1\Lambda_2)\,|\text{state}\rangle$$

So U provides representation acting in the Hilbert space. Further, changing the frame should preserve the norm of the state, so $U(\Lambda)$ should be unitary. We'll work out the form of this rep acting on one-part states explicitly, since we'll see that it is slightly subtle to get normalization right.

The obvious thing to do is define

$$U(\Lambda)\,|\vec{k}\rangle = |\Lambda\vec{k}\rangle$$

-- Lorentz transformation acting on particle with 4-momentum $(\omega_k, \vec{k}) = k$ boosts momentum to Λk. But this is not quite satisfactory because it is not unitary.

The states $|\vec{k}\rangle$ are normalized $\langle \vec{k}' | \vec{k}\rangle = \delta^3(\vec{k}-\vec{k}')$

and therefore $\mathbb{1} = \int d^3k \; |\vec{k}\rangle\langle\vec{k}|$ (completeness)

Now check $UU^+ = \mathbb{1}$

$$U\mathbb{1}U^+ = \int d^3k \;\; U(\Lambda)|\vec{k}\rangle\langle\vec{k}|U(\Lambda)^+$$

$$= \int d^3k \;\; |\Lambda\vec{k}\rangle\langle\Lambda\vec{k}|$$

$$= \int d^3(\Lambda^{-1}k)\;\; |\vec{k}\rangle\langle\vec{k}|$$

-- But the measure $d^3\vec{k}$ is not Lorentz invariant

The measure d^4k is Lorentz invariant, so we can write Lorentz invariant integral over 3-momentum in terms of

$$\frac{d^4k}{(2\pi)^3}\,\delta(k^2-m^2)\,\Theta(k^0)$$

picks out + $\sqrt{}$ of $\vec{k}^2+m^2$

$$= \frac{d^3k}{(2\pi)^3}\,\frac{1}{2\omega_k}$$

If we now introduce states

$$|k\rangle_{new} = (2\pi)^{3/2}\sqrt{2\omega_k}\;\;|\vec{k}\rangle_{old},$$

nonnorm

The new normalization is

$$ {}_{new}\langle k' | k \rangle_{new} = (2\pi)^3\, 2\omega_k\, \delta^3(\vec{k}' - \vec{k}) $$

— "Relativistic Norm."

and now

$$ \mathbb{1} = \int \frac{d^3k}{(2\pi)^3 2\omega_k} |k\rangle\langle k| $$

and therefore, if we define the action of U as

$$ U(\Lambda)|k\rangle = |\Lambda k\rangle, $$

then $U(\Lambda)$ is a unitary representation

We can write a relativistically normalized state as

$$ |k\rangle = \alpha^{+}(k)|0\rangle \qquad \alpha(k) = (2\pi)^{3/2}\sqrt{2\omega_k}\, a(\vec{k}) $$

then we can infer how $\alpha(k)$ transforms:

$$ U(\Lambda)|k\rangle = |\Lambda k\rangle = U(\Lambda)\alpha(k)^{+}U(\Lambda^{-1})|0\rangle $$

$$ = \alpha(\Lambda k)^{+}|0\rangle $$

vac is invariant

$$ \text{So} \quad U(\Lambda)\alpha(k)U(\Lambda)^{+} = \alpha(\Lambda k) $$

(evidently true not just acting on $|0\rangle$, but on any state)
And so we know how ϕ transforms:

$$ \phi(x) = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\left[e^{-ik\cdot x}\alpha(k) + e^{ik\cdot x}\alpha^{+}(k)\right] $$

$$ U(\Lambda)\phi(x)U(\Lambda)^{+} = \int \frac{d^3k}{(2\pi)^3 2\omega_k}\left[e^{-i(\Lambda^{-1}k)\cdot x}\alpha(k) + e^{i(\Lambda^{-1}k)\cdot x}\alpha^{+}(k)\right] $$

(since measure is invariant)
But Lorentz invariant inner product $\Rightarrow (\Lambda^{-1}k\cdot x) = (k\cdot\Lambda x)$
and thus $\quad U(\Lambda)\phi(x)U(\Lambda)^{+} = \phi(\Lambda x)$

and we see that ϕ transforms as a scalar field should under Lorentz transformations.

Notice that all the steps in this argument are reversible. We could start with the transformation property of $\phi(x)$, then infer how α and the relativistically normalized states transform. We thus find that quantization of scalar field yields spinless particles. (Spin zero means invariance under little group that leaves p invariant — a rotation in the zero momentum frame, or rotation about the $\vec{p}$ axis, for a massless particle)

Schrödinger Representation

For most applications of quantum field theory, it is convenient to use the Heisenberg representation, as noted previously. But it is of conceptual value to note that the Schrodinger picture can be used if desired. Then time evolution prescribes how states vary in time, states that can be described by "wave functionals". For example, the energy eigenstates in this picture are solutions to a functional Schrödinger equation.

Consider again the form of the Hamiltonian of the free scalar field in momentum space

$$H = \int d^3k \ \tfrac{1}{2}\left[\tilde{\pi}(\vec{k},t)\tilde{\pi}(-\vec{k},t) + \tfrac{1}{2}(\vec{k}^2+m^2)\tilde{\phi}(\vec{k},t)\tilde{\phi}(-\vec{k},t)\right]$$

$$[\tilde{\phi}(\vec{k},t), \tilde{\pi}(\vec{k}',t)] = i\delta(\vec{k}+\vec{k}')$$

When we write down the Schrodinger eqn

$$\left[-\frac{1}{2m}\vec{\nabla}^2 + V(\vec{q})\right]\psi(\vec{q}) = E\psi(\vec{q})$$

we have chosen to represent the Hilbert space in which $\vec{q}$ and $\vec{p}$ act as

$$\mathcal{H} = \{\text{(square integrable) functions of } \vec{q}\}$$

and the commutation relation $[q_i, p_j] = i\delta_{ij}$ is properly represented by

$$\vec{p} = -i\vec{\nabla} \qquad \text{(Schrödinger Rep.)}$$

To write down a functional Schrodinger eqn. in field theory, we choose

$$\mathcal{H} = \{\text{(square integrable) functionals of } \phi(\vec{k})\}$$

and represent the commutation relation by

$$\pi(\vec{k}) = -i\frac{\delta}{\delta\phi(-\vec{k})} \qquad \text{(operators have no time dependence in this picture)}$$

(I stopped writing squiggl,ies)

The Hamiltonian is thus represented by

$$H = \int d^3k\left[-\frac{1}{2}\frac{\delta}{\delta\phi(\vec{k})}\frac{\delta}{\delta\phi(-\vec{k})} + \frac{1}{2}\omega_k^2\phi(\vec{k})\phi(-\vec{k})\right]$$

and the schrödinger eqn can be written

$$H\,\psi[\phi(\vec{k})] = E\,\psi[\phi(\vec{k})]$$

By the same manipulations as before, we may write

$$H = \int d^3k\left[\omega_k a(\vec{k})^\dagger a(\vec{k}) + \text{constant}\right]$$

where
$$a(\vec{k}) = \frac{1}{\sqrt{2\omega_k}} \frac{\delta}{\delta\phi(-\vec{k})} + \sqrt{\frac{\omega_k}{2}}\,\phi(\vec{k})$$

E.g.
The ground state wave functional satisfies the first order eqn

$$a(\vec{k})\,\Psi = 0 \qquad (\text{for all } \vec{k})$$

-- and is therefore, up to normalization

$$\Psi[\phi(\vec{k})] = \exp\left[-\tfrac{1}{2}\int d^3k\ \omega_k\,\phi(\vec{k})\,\phi(-\vec{k})\right]$$

(i.e. $\prod_{\vec{k}} e^{-\frac{1}{2}\omega_k \phi(\vec{k})\phi(-\vec{k})}$

-- product of ground state wave function for each oscillator)

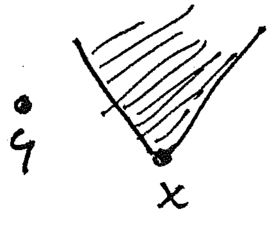
Causality (the algebra of observables)

We've constructed the Hamiltonian of the free scalar field, and found the energy eigenstates. But to complete the specification of the theory, we must also classify the set of observables of the theory -- quantities that can in principle be measured.

Of special interest are the local observables, those defined at a single spacetime point. For one thing, it is from the class of local observables that candidate interaction terms will be selected, if we wish to construct a theory of interacting particles.

Ordinarily (in nonrelativistic QM) all self-adjoint operators are observables, but in a relativistic theory there is a special restriction that comes from causality. Since information cannot propagate faster than c, a measurement at spacetime point x must not be able to influence a measurement at y if x, y have spacelike separation, $(x-y)^2 < 0$. Thus, for any two observables $\mathcal{O}_1$ and $\mathcal{O}_2$, we require

$$[\mathcal{O}_1(x), \mathcal{O}_2(y)] = 0 \quad , \text{for } (x-y)^2 < 0$$



(then arbitrarily accurate measurement of $\mathcal{O}_1$ at x does not preclude arbitrarily accurate measurement of $\mathcal{O}_2$ at y)

This is a defining property of the "algebra of observables" (algebra because operators come equipped with a commutator); if we admit $\mathcal{O}_1$ we cannot admit $\mathcal{O}_2$ unless the above condition is satisfied

It turns out that the allowed local observables $\mathcal{O}(x)$ are those that can be constructed as functions of the field ϕ and its derivatives at the point x. This is what you might have guessed, but the result is not trivial.

For example, recall that $\phi(x)$ -- the free scalar field, can be split into + and - frequency parts

$$\phi(x) = \phi^{(-)}(x) + \phi^{(+)}$$

$$\phi^{(-)}_{(x)} = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\, a(\vec{k})\, e^{-ik\cdot x}$$

$$\phi^{(+)}_{(x)} = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}}\, a(\vec{k})^+ e^{i\vec{k}\cdot\vec{x}}$$

(so $\phi^{(+)}$ and $\phi^{(-)}$ are hermitian conjugates)

Then it turns out that if we admit $\phi(x)$ to the algebra of local observables, then we cannot admit

$$\phi^{\theta}(x) = e^{-i\theta}\phi^{(-)}_{(x)} + e^{i\theta}\phi^{(+)}_{(x)},$$

although it is also a hermitian operator, for $e^{i\theta} \neq 1$. (We can construct a local algebra from either ϕ^{θ} or ϕ -- they differ by only a phase convention -- but not both.)

(Note that $\phi^{(-)}(x)$ is not a local function of $\phi(x)$. We have

$$a(\vec{k}) = \int \frac{d^3x'}{(2\pi)^{3/2}\sqrt{2\omega_k}} e^{ik\cdot x'}[i\dot{\phi}(x') + \omega_k \phi(x')],$$

so

$$\phi^{-}(\vec{x},t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \int d^3x' e^{i\vec{k}\cdot(\vec{x}'-\vec{x})} [i\dot{\phi}(\vec{x}',t) + \omega_k \phi(\vec{x}',t)]$$

$$= \tfrac{1}{2}\phi(\vec{x},t) + i\int d^3x' f(\vec{x}'-\vec{x})\, \dot{\phi}(\vec{x}',t)$$

where $f(\vec{x}) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{i\vec{k}\cdot\vec{x}}$)

To verify the above statements, consider the properties of the function

$$\Delta_+(x-y; m^2) \equiv [\phi^{(-)}(x), \phi^{(+)}(y)]$$

$$= \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{-ik\cdot(x-y)}$$

This is evidently a function of only the spacetime separation $x-y$ (translation invariance). Further, since the measure appearing in the integral is the Lorentz-invariant measure, we see

$$\Delta_+(\Lambda x) = \Delta_+(x)$$

-- the commutator is frame independent; reflecting that our quantization procedure did not destroy Lorentz invariance

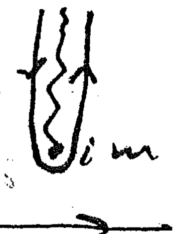
Furthermore, the function $\Delta_+(x)$ is certainly nonvanishing outside the light cone, $x^2 < 0$. If x is spacelike, we can choose frame with $x^0 = 0$ (remember, Δ_+ is frame-independent) then

$$\Delta_+(\vec{x}) = \int \frac{d^3k}{(2\pi)^3 2\sqrt{\vec{k}^2+m^2}} e^{i\vec{k}\cdot\vec{x}}$$

$$= \int \frac{dk\, k^2}{8\pi^2\sqrt{k^2+m^2}} \int_{-1}^{1} d\cos\theta\, e^{ikr\cos\theta}$$

$$= \frac{1}{8\pi^2 i r}\int_0^\infty \frac{dk\, k}{\sqrt{k^2+m^2}}\left(e^{ikr} - e^{-ikr}\right)$$

$$= \frac{1}{8\pi^2 i r}\int_{-\infty}^{\infty} \frac{dk\, k}{\sqrt{k^2+m^2}} e^{ikr}$$



Now, distort contour into upper half plane, obtaining contribution along the $\sqrt{\ }$ cut

$$= \frac{1}{8\pi^2 i r} 2\int_m^\infty \frac{i\,dz\; iz}{i\sqrt{z^2-m^2}} e^{-zr} \qquad (\text{sign?})$$

$$= \frac{m}{4\pi^2 r}\int_1^\infty \frac{z\,dz}{\sqrt{z^2-1}} e^{-z(mr)}, \text{ where } r = (-x^2)^{\frac{1}{2}}$$

Integrand has a definite sign, so this certainly doesn't vanish. (Actually, this is the integral rep of a modified Bessel function) the integral is obviously order e^{-mr}, so we see that Δ_+, though nonvanishing, becomes exponentially small many compton wavelengths outside the light cone.

It is amusing to note that this result has an interpretation in terms of particles propagating in spacetime. Since the commutator is a c-number (not an operator) it is the same as its expectation value in the vacuum (or in any other state) so

$$\Delta_+(x-y) = \langle 0| [\phi^{(-)}(x), \phi^{(+)}(y)] |0\rangle$$
$$= \langle 0| \phi^-(x)\, \phi^+(y) |0\rangle,$$

the second equality following because ϕ^- annihilates the vacuum. Now we can think of $\phi^+(y)$ as an operator that creates a particle localized at y, so $\Delta_+(x-y)$ may be interpreted as the amplitude for a particle created at $\vec{y}$ at time y^0 to propagate to $\vec{x}$ at time x^0

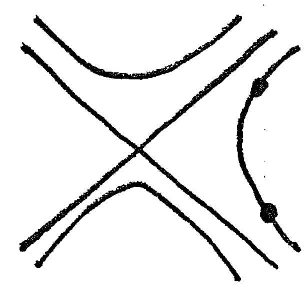
(this sounds a bit odd for $x^0 < y^0$ -- the particle is propagating back in time -- but the time-ordering is frame dependent anyway) So it appears that the particle has a nonzero amplitude to propagate faster than light.

But causality only requires that information cannot propagate faster than light, which brings us back to the algebra of observables. Now $\phi^{(-)}$ and $\phi^{(+)}$ are not observable, so consider the hermitian combination

$$\phi(x) = \phi^{(-)}(x) + \phi^{(+)}(x)$$

$$i\Delta(x-y;m^2) = [\phi^{(-)}(x)+\phi^{(+)}(x),\ \phi^{(-)}(y)+\phi^{(+)}(y)]$$
$$= \Delta_+(x-y) - \Delta_+(y-x)$$

This vanishes outside the light cone if $\Delta_+(x)$ is an even function outside the light cone. But it is, because Δ_+ is Lorentz invariant, and if $x^2<0$, there is always a Lorentz transformation (boost) that takes



$$(x^0,\vec{x}) \text{ to } (-x^0,-\vec{x})$$

(This is not true for $x^2 \geq 0$ -- we can't change the sign of x^0 with a boost -- and Δ will not vanish. -- Problem is the $\theta(k^0)$ in the Lorentz invariant measure)

oscillating Bessel function

On the other hand

$$[\phi^\theta(x), \phi(y)] = e^{-i\theta}\Delta_+(x-y) - e^{i\theta}\Delta_+(y-x)$$
$$= -2i\sin\theta\,\Delta_+(x-y)$$

outside light cone, so ϕ^θ cannot be admitted to the algebra of local observables (unless $\sin\theta = 0$).

Consider the spacetime interpretation of what we have done:

$$\langle 0|[\phi(x),\phi(y)]|0\rangle = \langle 0|\phi^-(x)\,\phi^+(y)|0\rangle - \langle 0|\phi^-(y)\,\phi^+(x)|0\rangle$$

We have achieved causality through a subtle interference effect!

Outside the light cone, the amplitude for propagation (forward in time) from x to y is cancelled by the amplitude for propagating (backward in time) from y to x. Both amplitudes must be present in a causal theory. (Later, we'll see that this requires the existence of antiparticles, and gives rise to the connection between spin and statistics)

Of course, if $\phi(x)$ and $\phi(y)$ commute for spacelike separation, then so do derivatives of ϕ; e.g.

$$[\partial_\mu \phi(x), \phi(y)] = \partial^x_\mu \Delta(x-y)$$

-- and functions of ϕ and its derivatives.

Incidentally, in keeping with the spacetime interpretation (and for other reasons), it is often convenient to introduce the function

(check for i's) $$i\Delta_F(x-y) = \langle 0|\, \text{`}T\text{'}[\phi(x)\,\phi(y)]\,|0\rangle$$ = "Feynman Propagator"

where 'T' denotes time ordering:

$$\text{`}T\text{'}[\phi(x)\phi(y)] = \theta(x^0-y^0)\,\phi(x)\phi(y) + \theta(y^0-x^0)\,\phi(y)\phi(x)$$

(Later times to the left, earlier to the right) this picks out the amplitude for propagation from the earlier time to the later time -- and is nonvanishing outside the light cone. Properties of

$$i\Delta_F(x) = \theta(x^0)\,\Delta_+(x) + \theta(-x^0)\,\Delta_+(-x)$$

are to be worked out in the exercises.

Now, we are in a much better position to understand why, desiring a theory of free (spin 0) particles, we began by considering a theory of free (scalar) fields.
If we had the notion that particles are the fundamental entities, we would begin with a Fock space -- a Hilbert space spanned by n-particle states of the form

$$|\vec{k}_1, \text{--} \vec{k}_n\rangle$$

(where all particles have spin 0, mass m, and the energy is $\sum \omega_K$). But suppose that, in this theory of free particles, we wanted to define local observables. (We would want local observables if, for example, we wanted to introduce local interactions.) How would we proceed?

We could introduce operators $\alpha(K), \alpha(K)^+$ that destroy, create relativistically normalized one-particle states:

$$|K\rangle = \alpha(K)^+|0\rangle$$

then the Hilbert space is spanned by powers of α^+ acting on $|0\rangle$.

Next, we would try to introduce an object $\phi(x)$ with the properties:

(i) $U(\Lambda, x_0)\,\phi(x)\,U(\Lambda, x_0)^{-1} = \phi(\Lambda x + x_0)$

where
$U(\Lambda, x_0)|K\rangle = e^{i\Lambda K \cdot x_0}|\Lambda K\rangle$ (transforms as a scalar under Poincaré transformations)

(ii) $[\psi(x), \psi(y)] = 0$ for $(x-y)^2 < 0$

(so ψ is a local observable)

(iii) $\psi(x)$ is linear in α and α^+
(assumed so that ψ will be the simplest nontrivial local observable)

The most general object that satisfies these conditions (and is hermitian) is

$$\psi(x) = c\,\phi^{\theta}(x)$$

It is just the free scalar field, up to the real normalization constant c, and the phase $e^{-i\theta}$ in $\phi^{(-)}$ which can be absorbed in a change of the phase convention for α. Further, once $\phi(x)$ is admitted to the algebra of observables, we know that $\phi^{\theta}(x)$ cannot be admitted, for $e^{i\theta} \neq \pm 1$

Since ϕ satisfies the Klein-Gordon field eqn, we have been inexorably led back to the free scalar field theory!
(The K-G eqn follows from the "mass-shell condition" $p^2 = m^2$ for the free particles.)

Measurement of Quantum Fields (Uncertainty Relations)

We have stressed several times that the field $\phi(x)$ is an "observable." This means that we can conceive of measuring it. Furthermore, the commutator $[\phi(x), \phi(y)]$, which is nonvanishing inside the light cone, indicates the fundamental limitation on such measurements. We cannot in general measure both $\phi(x)$ and $\phi(y)$ to arbitrary accuracy.

Similar limitations arise in ordinary nonrelativistic QM. In that case, it is possible to acquire an intuitive understanding of these limitations: Heisenberg's "microscope" demonstrates why a precise determination of position necessarily generates a large uncertainty in momentum. We would like to extend that intuition to quantum fields — to understand these new limitations in terms of Heisenberg's microscope.

For this purpose, I'll consider the $m^2 \to 0$ limit of our free scalar field theory, for two reasons:
i) the mathematics is simpler
ii) Our scalar mesons are then massless, like photons, and some of our intuition about electrodynamics then applies.

In the $m^2 = 0$ case, it is easy to write down an explicit expression for the field commutator:

$$[\phi(x),\phi(y)] = \Delta_+(x-y;m^2) - \Delta_+(y-x;m^2) = i\Delta(x-y;m^2)$$

where $\Delta_+(x;m^2) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{-ik\cdot x}$

And, for $m^2=0$, $\omega_k = |\vec{k}|$, and we have

$$i\Delta(x) = \int_0^\infty \frac{dk\,k^2}{8\pi^2 k}\left(e^{-ikt}-e^{ikt}\right)\int_{-1}^{1} d\cos\theta\, e^{ikr\cos\theta}$$

$$= \frac{1}{8\pi^2 ir}\int_0^\infty dk\, \underbrace{\left(e^{-ikt}-e^{ikt}\right)\left(e^{ikr}-e^{-ikr}\right)}_{[e^{ik(r-t)}+e^{-ik(r-t)}-e^{ik(r+t)}-e^{-ik(r+t)}]}$$

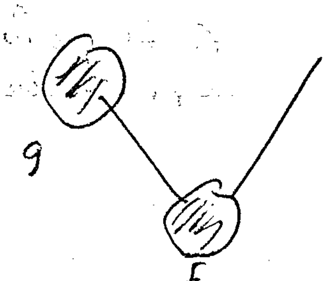
$$i\Delta(x) = \frac{-i}{4\pi r}\left[\delta(r-t)-\delta(r+t)\right]$$

Thus we see that, in the case $m^2=0$, the commutator has its support only on the light cone.

(Note: to check this, take

$$\frac{\partial}{\partial t} i\Delta(x)\Big|_{t=0} = [\dot\phi(\vec{x},0),\phi(\vec{0},0)] = \frac{i}{2\pi r}\delta'(r)$$

this is in agreement with canonical commutator, since RHS is $-i\delta^3(\vec{x})$ in spherical coordinates)



Evidently then, measurements of $\phi(f)$ and $\phi(g)$ -- fields smeared in spacetime -- cannot both be made to arbitrary accuracy, if there are points in support of f and g with lightlike separation.

To understand this result, we must think about how a measurement of the field ϕ might be performed. For guidance, think of electrodynamics. How do we measure electric field $\vec{E}$? We introduce a charged test particle, and measure the ratio of mass×acceleration to charge:

$$\vec{F} = m\vec{a} = q\vec{E}$$

Now, the same method ought to be applicable to the massless free scalar field. Indeed, the value of ϕ itself is purely conventional, since $\phi \to \phi + \text{constant}$ is a symmetry of the massless theory; the interesting quantity to measure is gradient of ϕ. So imagine that we couple $\phi(x)$ to an "external" distribution of charge, which is to be treated classically. The action becomes

$$S = \int d^4x \left[\tfrac{1}{2}\partial_\mu\phi\,\partial^\mu\phi + J(x)\phi(x) \right]$$

Thus, $-\phi(x)$ is the "potential" for the charge density $J(x)$

$$H_{new} = -\int d^3x\, J\phi$$

and the force on a test body with charge

$$Q = \int_V d^3x\, J$$

is

$$\vec{F} = Q\vec{\nabla}\phi$$

To measure the value of $\vec{\nabla}\phi$ averaged over spacetime volume VT, we take a test particle with volume V and charge Q and measure the impulse it receives from the field $\vec{\nabla}\phi$ over a time T. We have

$$\delta\vec{p} = QT\vec{\nabla}\phi$$

The uncertainty in our measurement of $\vec{\nabla}\phi$ is linearly related to the accuracy of our measurement of the impulse, and therefore inversely related to our uncertainty about the position of the test particle:

$$\Delta(\nabla_i\phi) = \frac{1}{QT}\Delta(\delta p_i) = \frac{\hbar}{QT\Delta(x_i)}$$

We see that a very accurate measurement of $\nabla\phi$ necessarily involves large uncontrollable fluctuations in the position of the test charge. And this suggests an interpretation of the uncertainty relations for field measurements. An accurate measurement of $\nabla\phi$ at one place induces fluctuations of the test body. But a fluctuating charged body radiates. And the radiation gives rise to uncontrollable effects on the field elsewhere (on the light cone, in the massless case, since radiation travels at speed c).

Let's see if this conjectured interpretation will hold up quantitatively. (It should agree with the limitations implied by the field comm. relations.)

We need to know how the fluctuating test charge influences the field elsewhere. For this purpose, we'll treat the reaction of the field classically. This is an approximation that should be valid if there are many field quanta involved, something we can check later.

In the presence of a charge distribution, the classical field equation becomes

$$\Box \phi(x) \equiv \left(\frac{\partial^2}{\partial t^2} - \vec{\nabla}^2\right) \phi(x) = J(x)$$

The solution to this equation can be found by the Green function method:

$$\phi(x) = \int d^4x' \, G(x-x') \, J(x')$$

where G satisfies

$$\Box_x G(x-x') = \delta^4(x-x')$$

and the appropriate boundary condition. We want a causal soln, so we use the retarded Green function:

$$G^{ret}(x-x') = \frac{1}{4\pi|\vec{x}-\vec{x}'|} \delta(t'-t+|\vec{x}-\vec{x}'|)$$

-- i.e. an initial point source propagates radially outward and forward in time, while amplitude falls like $\frac{1}{r}$ -- the familiar behavior of a causal soln to the wave eqn.

Let $x_1 = (\vec{x}_1, t_1)$ be the spacetime position of a fluctuating charge, which fluctuates during a time interval T. Then the response of the field at x_2 is

$$\phi(\vec{x}_2, t_2) = \int d^4x' J(x') \frac{1}{4\pi|\vec{x}_2 - \vec{x}'|} \delta(t' - t_2 + |\vec{x}_2 - \vec{x}'|)$$

$$= QT \frac{1}{4\pi|\vec{x}_2 - \vec{x}_1|} \delta(t_1 - t_2 + |\vec{x}_2 - \vec{x}_1|)$$

(there is an implicit averaging here over the volume of the fluctuating charge and the time T)

Now suppose $\vec{x}_1 = \vec{x}_1^{\,0} + \Delta\vec{x}_1$ where $\Delta\vec{x}_1$ is a fluctuation to be regarded as small compared to the separation of 1 and 2. Then in linear order, we have

$$\Delta\phi(x_2) = QT(\Delta x_1)_i \frac{\partial}{\partial x_1^i} \frac{1}{4\pi|\vec{x}_2 - \vec{x}_1|} \delta(t_1 - t_2 + |\vec{x}_2 - \vec{x}_1|)$$

(This is the fluctuation in $\phi(x_2)$ due to i-component of $\Delta\vec{x}$) But

$$QT(\Delta x_1)_i = \frac{\hbar}{\Delta(\nabla_i \phi(x_1))}$$

Actually, we should expand in Δx first, then average over T.)

So we have

$$\Delta(\nabla_i \phi(x_1))\,\Delta(\nabla_j \phi(x_2))$$

$$= \hbar \frac{1}{4\pi} \frac{\partial}{\partial x_2^j} \frac{\partial}{\partial x_1^i} \frac{1}{4\pi|\vec{x}_2 - \vec{x}_1|} \delta(t_1 - t_2 + |\vec{x}_2 - \vec{x}_1|)$$

The properties of the test charge drop out here -- this is an intrinsic property of field measurements.

This is in perfect agreement with our expectation based on the field commutator:

$$[\nabla_i \phi(x), \nabla_j \phi(y)] = \frac{\partial}{\partial x^i}\frac{\partial}{\partial y^j}\, i\Delta(x-y)$$

Fluctuations of $\phi(x)$

Since a destroys particles and $a^\dagger$ creates particles, the free scalar field has vanishing expectation value in the vacuum:

$$\langle 0|\, \phi(x)\, |0\rangle = 0$$

The same applies to the expectation value in any state with a definite number of particles. Thus, the mean value of measurements of $\phi(x)$ in the vacuum is zero.

But how large are the fluctuations in $\phi(x)$ in e.g. the vacuum state?

Using

$$\phi(x) = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \left[a(k)e^{-ik\cdot x} + a(k)^\dagger e^{ik\cdot x}\right]$$

we compute

$$\langle 0|\, \phi(x)^2 |0\rangle = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \int \frac{d^3k'}{(2\pi)^{3/2}\sqrt{2\omega_{k'}}}\, e^{-i(k-k')\cdot x} \langle 0|a(k)a(k')^\dagger|0\rangle$$

$$= \int \frac{d^3k}{(2\pi)^3}\, \frac{1}{2\omega_k}$$

-- This is (ultraviolet) divergent

the fluctuations of $\phi(x)$ are actually infinite. And this is evidently also true in any Fock space state with a definite (finite) no. of particles.

What we have found is an apparent incompatibility between detecting particles and measuring fields. A measurement of ϕ at the spacetime point x requires perfect resolution and hence infinite energy. Such a measurement involves the production of an indefinite number of particles.

We've also found another indication that quantum fields must be regarded as operator-valued "distributions" -- they must be "smeared" against suitable test functions (in space or in space and time) in order to make sense.

If we define a smeared field

$$\phi(f,t) = \int d^3x \; \phi(\vec{x},t) f(\vec{x})$$

then

$$\langle 0|\, \phi(f,t)^2 \,|0\rangle = \int d^3x\, d^3x' \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\omega_p} e^{-ip\cdot x} e^{ip\cdot x'}$$

$$= \int d^3p \; \frac{f(\vec{p}) f(-\vec{p})}{2\omega_p} = \int d^3p \; \frac{|f(\vec{p})|^2}{2\omega_p}$$

-- which is finite if $f(\vec{p})$ is rapidly decreasing.

For example, if $f(\vec{p})$ is a gaussian with width $\Lambda \gg m$, we have

$$\langle \phi(f)^2 \rangle \sim \Lambda^2$$

then $f(\vec{x})$ has width Λ^{-1}. So fluctuations of ϕ are order Λ, inverse size of region over which ϕ is smeared.

In order for a field strength averaged over a region to be considered "classical" it must be large compared to fluctuations of ϕ.