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QFT in Curved Spacetime

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1 Introduction

A typical first-year graduate student may take a year-long course on general relativity and a year-long course on advanced (relativistic) quantum mechanics. Most likely, they hear little about quantum theory in the GR course and little about gravity in the QFT course. Why?

There are practical reasons. Experts in GR are often not experts in QFT, and vice versa. Most interesting physics applications of GR concern phenomena on long-distance scales where QFT has little relevance - the structure and evolution of the universe, relativistic astrophysics, and astrophysical black holes, sources of gravitational radiation. Likewise, the exciting physics applications of QFT typically cover phenomena at very short distances, such as particle-particle collisions. These applications fail to provide a context in which gravity and quantum theory need to be considered simultaneously.

In what sort of context are GR and QFT simultaneously relevant?

A first hint was actually provided in 1899 by Planck, who noticed that the fundamental constants $\hbar$, along with c and Newton's constant G allow us to construct fundamental units of distance, time, energy, etc...

Distance: $L_p = \left(\frac{G\hbar}{c^3}\right)^{\frac{1}{2}} \sim 10^{-33}$ cm
Time: $T_p = \frac{L_p}{c} = \left(\frac{G\hbar}{c^5}\right)^{\frac{1}{2}} \sim 10^{-43}\,\mathrm{sec}$
Energy: $E_p = \frac{\hbar}{T_p} = \left(\frac{\hbar c^5}{G}\right)^{\frac{1}{2}} \sim 10^{19}\mathrm{GeV}$
Just on dimensional grounds, then, one expects that gravity and quantum theory are relevant for phenomena at distances $\sim L_p$ or energies $\sim E_p$.

To be more concrete, consider the gravitational contribution to hard (large-angle) scattering between relativistic particles. Merely on dimensional grounds, the cross-section $\sigma \sim G^2E^2 \quad (\hbar = c = 1)$.

This becomes appreciable (comparable to the "unitarity limit" $\sim 1/E^2$) for $E \sim E_p \sim 10^19$GeV. At such energies quantum quantum corrections higher order in $\hbar$ become important. These corrections turn out to be so sensitive to the nature of quantum fluctuations with $\omega \geq E_P$ that the calculability of the theory breaks down. (Einstein's gravity is nonrenormalizable). This breakdown of caulculability at $E \sim E_P$ can indication rhat Einstein gravity must be replaced by a more complete underlying theory (Superstring theory?)

The breakdown of Einstein gravity at $L \sim L_P$ is more profound than say, the breakdown of Fermi's weak interaction theory at $E \approx 300$ GeV. For the dynamical variable of quantum gravity is the spacetime metric itself. Large quantum fluctuations may turn the whole notion of spacetime upside down. At the very least, it is obscure how to formulate microscopic causality for a theory in which the edge of the lightcone is broad and fuzzy.

Quite aside from the ambiguities that afflict quantum gravity at "short distances," there are deep conceptual questions concerning the interpretation of a quantum theory of gravity – these stem from the genreral covariance of the theory. In general relativity, the coordinates that parametrize spacetime have no invariant significance, and so we are free to reparametrize spacetime locally. Whenever we formulate quantum mechanics, we must (*arbitrarily*) choose a time coordinate t and construct a Hamiltonian H that generates time evolution. Now we should distinguish two types of reparametrizations, which have quite distinct physical consequences:

1. We can reparametrize *each* time slice t = constant. This is an example of gauge invariance – it is a redundancy in how the metric ${}^3g$ of the time slice parametrizes the quantum states, like the redundancy in how the vector potential A_μ of electrodynamics parametrizes states.. The "wave function" $\psi\left({}^3g\right)$ must be regarded as a functional of the 3-geometry represented by the metric, not the metric itself.

2. We can reparametrize time, or choose a new set of time slices. Because we have the freedom to move the time slice forward or backward locally, the quantum theory will not tolerate *any* time-dependence:

   $i\frac{\partial\psi}{\partial t} = H\psi = 0.$

   This is the Wheeler-DeWitt equation.

So, naively, the theory has no dynamics, at least with respect to the extrinsic *parameter* time. To formulate dynamics, we must identify an intrinsic time. We ask not "What is $P(x,t)$, the probability that the electron is at x at 12 noon"
but
"What is $P(x/t)$, the conditional probability that the electron is at x when the clock says t."

The change is not trivial because if time is the reading of a clock itself is a quantum-mechanical dynamical variable, then time itself is subject to quantum fluctuations.

Without a meaningful extrinsic time, it is not clear how we are to construct a self-consistent probability interpretation of quantum mechanics. What we ordinarily do is choose a complete set of commuting observables and consider $|\lambda, t\rangle$ that are eigenstates of all these observables at time t. Then, $P(\lambda, t) = |\langle\lambda, t|\psi\rangle|^2$ is the probability distribution for a measurement of the observables. It satisfies a normalization property:

$$\sum_\lambda P(\lambda, t) = \sum_\lambda \langle \psi | \lambda, t \rangle \langle \lambda, t | \psi \rangle$$
$$= \langle \psi | \psi \rangle = \mathbb{1}$$

because the observables are complete.

Because of the "problem of time" in general relativity, it is not clear how to construct a complete set of observables that obey conservation in probability. There is a "semiclassical" limit in which fluctuations in time can be ignored and the normal theory applies, but we would like quantum gravity to have an interpretation beyond semiclassical theory. (And what ensures that semiclassical behavior is ever attained?)

Thus, because of the problem of time, we do not yet understand whether quantum gravity has a fully consistent probability interpretation. This is a deep conceptual problem, quite independent of the short-distance problem.

$$\text{But } E \sim E_P \sim 10^{19}\text{GeV}, L \sim L_P \sim 10^{-33} \text{ cm}$$

seems so remote from all experience, should we really care about such issues? The motivation to understand quantum gravity arises from

1. The problem of initial conditions of the universe – "Quantum cosmology"
2. What is the final state of an evaporating black hole? (Does quantum mechanics break down?)
3. The hope that a better understanding of quantum gravity will elucidate physics in unexpected ways, including consequences more directly related to experiments.

Although we have argued that understanding quantum gravity is important, we will not be quite so ambitious in this course. In the hope of avoiding the conceptual quagmire described above, we will mostly focus on the regime where $L \gg L_P$ and $E \gg E_P$. In this regime, it is an excellent approximation to do quantum field theory but treat gravity as classical.

E.g. in Z^0 decay $Z- > \mu^+\mu^- +$ hard graviton gives a contribution that is suppressed by $\sim Gm_z^2 \sim 10^{-34}$ to the total Z width – Gravity is negligibly weak at low energy. The nonrenormalizability of quantum gravity does not alter this conclusion.

The long quantum fluctuations of $L \sim L_P$ *decouple* from the long-distance physics - except for effects that can be absorbed into renormalizing a few free parameters. This decoupling is what makes low-wavelength physics possible - without it, quantum field theory, and physics, would not be possible at all.

In this course, we will focus on the effect of *classical* gravity on the quantum theory of other fields – in other words, we will consider quantum field theory on a spacetime background with curvature that non-zero, but small in Planck units. The curvature significantly affects the excitations and fluctuations of the fields on wavelengths comparable to the scale set by the curvature.

By considering this limit, we will not avoid all subtleties and ambiguities. For example, the notion of a particle is difficult to make precise on a curved background. Correspondingly, it will not always be obvious how to define a "vacuum" state of the quantum fields, or how to construct a Hilbert space built on the vacuum. These are features not encountered in classical GR or in QFT on flat spacetime, and we will need some ingenuity and pragmatism to deal with them.

Further subtleties arise when we consider the backreaction of quantum fields on the spacetime metric. It is simply not consistent to say that the quantum fields other than gravity, fluctuate – for these fields are a *source* for gravity. In a zeroth-order approximation, we may regard $\langle\psi\,|T_{\mu\nu}|\,\psi\rangle$ as a source of backreaction, but this is reasonable only if the fluctuations in $T_{\mu\nu}$ are small enough so that they will only perturb the geometry only a little. And it is not easy to decidee how the operator $T_{\mu\nu}$ appearing in the expectation value is to be quantized.

Our main objective in this course is to understand the classic applications of quantum field theory in curved spacetime:

- Black Hole Radiation - The key to understanding the thermodynamics and entropy of black holes, as well as the (potential) loss of quantum coherence.
- Quantum Fluctuations in de Sitter Space - Perhaps the origin of primordial density fluctuations in the early universe that seeded galaxy formation, in the inflationary universe scenario.

  In attempting to grasp the above applications, it will also be enlightening to consider
- Rindler Space - The thermal radiation seen in the vacuum by a uniformly accelerated observer.

(In all these cases, we will be able to discuss the essential features by considering *free* quantum fields with zero spin.)

The essential feature that all three examples have in common is an *event horizon.*

We will also consider the backreaction – how the quantum fields act as source for the spacetime geometry, and how the stress-energy tensor is to be defined as a quantum mechanical operator.

2 Quantum Field Theory in Flat Spacetime

We will consider how quantum theory is reconciled with special relativity. That is, we wish to construct a quantum theory such that:

(i) Physics is frame-independent (Lorentz invariant).
(ii) Relativistic causality is respected (No propagation of information at $v > c$).

We note to begin with that there is a certain tension between the principles of quantum theory and of relativity. The uncertainty principle causes a localized wave packet to spread quickly. What will prevent probability from leaking out of the light cone? (And thus, information would propagate backward in time, in some frames.) It will turn out that causality requires a rather subtle conspiracy.

We are accustomed to the notion that symmetries in physics simplify physical problems. Thus, we might expect relativistic quantum theory - quantum theory constrained by Lorentz invariance - to be simpler than non-relativistic quantum mechanics. This expectation turns out to be a bit too naive. The reason is that, in a relativistic theory, particle production is possible, and, in fact, an indefinitely large number of particles can, in principle, be produced at sufficiently high energy. Therefore, relativistic quantum theory is inevitably a quantum theory with an infinite number of degrees of freedom. When we formulate perturbation theory, all possible states in the theory can appear as intermediate states. In a theory with an infinite number of degrees of freedom, we typically find:

- The perturbation theory is complicated.
- Perturbation theory suffers from (ultraviolet) divergences. Much of the subtlety of (relativistic) quantum field theory stems from these divergences. We need to understand their origin and how to deal with them.

Particles:

We wish to construct a quantum theory of non-interacting relativistic particles. How should we proceed? There are two basic strategies, complementary to one another.

1. Begin with a Hilbert space of relativistic particle states. Then introduce *fields* in order to construct observables that are localized in spacetime. This is called (for obscure reasons) "second quantization."
2. Begin with a relativistic (Lorentz invariant) classical field theory. Construct a quantum mechanical Hilbert space by elevating the field to the status of an operator that obeys

canonical commutation relations with its conjugate momentum. This is called "canonical quantization." One then finds relativistic particles in the spectrum of this theory.

Adopting either starting point, we are eventually led to the same theory. Strategy (1) is more crucial and direct if our initial objective is to obtain a theory of particles. But (2) is reasonable if our goal is to construct a quantum theory with relativistically invariant (and causal) dynamics. Furthermore, when particles interact, the concept of a particle becomes ambiguous, and the advantages of (2) become more apparent.

Also, if spacetime is curved, the concept of a particle is again ambiguous, which leads me to favor (2). But we will see that (2) also suffers from ambiguities in curved spacetime. These ambiguities, whether (1) or (2) is used, in a spacetime that is curved, are central conceptual problems in the theory of quantum fields on curved spacetime.

We will describe procedure (1) in some detail and then (2) somewhat more schematically. Then we will go on to try to apply these procedures to field theory on a nontrivial background.

Notation: We will usually set $\hbar = c = 1$. Our spacetime metric will be of the form:

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

- following the conventions used by Birell and Davies.

To a particle theorist on a flat background spacetime (like me), a relativistic particle is a unitary irreducible representation of the Poincaré group. The Poincaré group is the semidirect product of the Lorentz group and translation group.

Lorentz transformation:

$$\Lambda : x^\mu \to \Lambda^\mu_\nu x^\nu$$

$$\eta_{\mu\nu}\Lambda^\mu_\lambda \Lambda^\nu_\sigma = \eta_{\lambda\sigma}$$

(We will always consider Λ to be a proper Lorentz transformation with $\Lambda^0_0 > 0$, and $\det \Lambda = 1$; these are Lorentz transformations that can be smoothly connected to the identity. That is, parity and time reversal are excluded.)

Translation:

$$a : x^\mu \to x^\mu + a^\mu$$

The Poincaré transformation (Λ, a) acts as

$$(\Lambda, a) : x \to \Lambda x + a.$$

Thus, the composition law for Poincaré transformations is:

$$(\Lambda_1, a_1) \cdot (\Lambda_2, a_2) = (\Lambda_1\Lambda_2, \Lambda_1 a_2 + a_1)$$

$$x \to \Lambda_2 x + a_2 \to \Lambda_1\Lambda_2 x + \Lambda_1 a_2 + a_1$$

Now, consider a quantum theory that respects Poincaré invariance. It has a Hilbert space, denoted as H, and unitary operators that represent Poincaré transformations acting on H:

$$(\Lambda, a) : |state\rangle \longrightarrow U(\Lambda, a)|state\rangle.$$

U is required to be unitary to preserve the inner product: $(\psi, \chi) = (U\psi, U\chi)$. This is what it means for Poincaré transformations to be symmetries.

Suppose we change reference frames twice:

$$\begin{aligned} |state\rangle &\to U(\Lambda_1, a_1)U(\Lambda_2, a_2)|state\rangle \\ &= U(\Lambda_1\Lambda_2, \Lambda_1 a_2 + a_1)|state\rangle \end{aligned}$$

For consistency, this must be equivalent to:

$$U(\Lambda_1, a_1)U(\Lambda_2, a_2) = U\left((\Lambda_1, a_1) \cdot (\Lambda_2, a_2)\right)$$

This is what it means to say that the unitary operator U's provides a representation of the Poincaré group.

What is the structure of such a representation? First, consider translations $(\mathbb{1}, a)$. Translations are generated by the momentum operator:

$$U(a) = e^{iP\cdot a}$$

The translation group is abelian, and its irreducible representations are one-dimensional. An irreducible representation actis on a state that is a simultaneous eigenstate of all components of P^μ:

$$P^\mu|k\rangle = k^\mu|k\rangle$$

Or

$$U(a)|k\rangle = e^{ik\cdot a}|k\rangle.$$

$|k\rangle$ is called the plane wave state. Clearly, $U(a_1)U(a_2) = U(a_1 + a_2)$, so this is a representation. (If we wish to think of k^μ as the four-momentum of a particle, note that $\hbar$ has already implicitly entered the discussion.)

How shall Lorentz transformations be represented? Let's consider the simplest case, where a state with $\vec{k} = 0$ is invariant under rotations ("spin 0"). If we think of $|k\rangle$ as a particle with four-momentum k^μ, then we expect that the state $U(\Lambda)|k\rangle$ should have momentum Λk. Indeed, this is required by the Poincaré group structure:

$$\begin{aligned} &U(\Lambda^{-1})e^{iP\cdot a}U(\Lambda) = U(\mathbb{1}, \Lambda^{-1}a) \\ \Rightarrow\ &U(\Lambda^{-1})e^{iP\cdot a}U(\Lambda) = e^{iP\cdot(\Lambda^{-1}a)} = e^{i\Lambda P\cdot a} \\ \Rightarrow\ &U(\Lambda^{-1})PU(\Lambda) = \Lambda P \end{aligned}$$

So $PU(\Lambda) = U(\Lambda) \cdot (\Lambda P)$, so that

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

Our representation of the translation group becomes a representation of the Poincaré group if we choose:

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

up to a normalization to be discussed in a moment.

The Lorentz transformations preserve the invariant:

$$P^\mu P_\mu = m^2;$$

and for our representation to correspond to physical particles, we demand:

$$m^2 \geq 0 \text{ and } P^0 \geq 0$$

Then, the states $|k\rangle$ with $k^2 = m^2$ and $k^0 > 0$ are the basis for an *irreducible* representation of the Poincaré group: Any k on the mass hyperboloid can be obtained from $k = (m, \vec{0})$ by applying a suitable Lorentz transformation.

The relative normalization of the state $|k\rangle$ for various values of k can be determined from the requirement that $U(\Lambda)$ defined by:

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

is a unitary operator. Because the states $|k\rangle$ form a complete basis for the representation space, we have:

$$\mathbb{1} = \int d\mu(k)|k\rangle\langle k|$$

for a suitable measure $d\mu$ defined on the hyperboloid. If U is unitary, then:

$$\begin{aligned} \mathbb{1} = U(\Lambda)\mathbb{1}U(\Lambda)^\dagger &= \int d\mu(k)U(\Lambda)|k\rangle\langle k|U(\Lambda) \\ &= \int d\mu(k)|\Lambda k\rangle\langle\Lambda k| = \int d\mu\left(\Lambda^{-1}k\right)|k\rangle\langle k| \end{aligned}$$

Thus, $d\mu(k)$ must be a *Lorentz invariant measure* satisfying:

$$d\mu(k) = d\mu\left(\Lambda^{-1}k\right)$$

The invariant measure is unique up to an overall multiplicative factor and can be written as:

$$d\mu(k) = \frac{d^4k}{(2\pi)^3}\delta\left(k^2 - m^2\right)\theta\left(k^0\right)$$

The measure d^4k is invariant because $\det\Lambda = 1$. Then, $\delta\left(k^2 - m^2\right)$ restricts this measure to the hyperboloid, and the $\theta\left(k^0\right)$ further restricts it to the positive energy hyperboloid. The $(2\pi)^{-3}$ is a convention that fixes the overall normalization.

Since k^0 can be trivially integrated, we may also write:

$$d\mu(k) = \frac{d^3k}{(2\pi)^3 2k^0}, \text{ where } k^0 = +\sqrt{\vec{k}^2 + m^2}$$

From

$$\mathbb{1} = \int \frac{d^3k}{(2\pi)^3 2k^0} |k\rangle\langle k|$$

and

$$\mathbb{1}\left|k'\right\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0} |k\rangle\left\langle k \mid k'\right\rangle = \left|k'\right\rangle,$$

we find the relativistic normalization of states:

$$\left\langle k' \mid k\right\rangle = (2\pi)^3 2k^0 \delta^3(\vec{k'} - \vec{k})$$

We have now completely specified the basis for the one-particle subspace $\mathcal{H}^{(1)}$ of Hilbert space in a theory of relativistic particles and have defined the action of the Poincaré group on this space. It acts irreducibly. The states in $\mathcal{H}^{(1)}$ are wave packets that can be expanded in terms of the plane wave basis eg:

$$|\tilde{f}(k)\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0} \tilde{f}(k)|k\rangle$$

where

$$U(\Lambda)|\tilde{f}(k)\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0} \tilde{f}(k)|k\rangle = \left|\tilde{f}\left(\Lambda^{-1}k\right)\right\rangle$$

and

$$\langle\tilde{f}'|\tilde{f}\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0} \tilde{f}'(k)^* \tilde{f}(k)$$

.

(Note: There is a natural conjugate basis:

$$|x\rangle = \left|\tilde{f} = e^{ik\cdot x}\right\rangle$$

such that

$$U(a)|x\rangle = \left|\tilde{f} = e^{ik\cdot(x+a)}\right\rangle = |x+a\rangle$$
$$U(\Lambda)|x\rangle = \left|\tilde{f} = e^{i\left(\Lambda^{-1}k\right)\cdot x}\right\rangle = |1x\rangle$$

But in this basis, the inner product is:

$$\langle x|x'\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0} e^{-ik\cdot(x-x')}$$

A Lorentz invariant quantity that does not vanish for any value of $x - x'$. The significance of this will be discussed below.)

We have constructed a one-particle Hilbert space, but in anticipation of interactions that might change the number of particles (E.g. - measurements), we will enlarge it to a many-particle Hilbert space.

First, we need a vacuum – the zero-particle state. It is the unique state that is Poincaré invariant:

$$P^\mu|0\rangle = 0 \qquad U(\Lambda)|0\rangle = 0$$

.

That is, the vacuum looks the same to all observers.

And we need many-particle states. We *assume* that the particles obey Bose statistics, e.g.:

$$|k_1, k_2\rangle = |k_2, k_1\rangle$$

So, the normalization of the n-particle state $|k_1, k_2, \ldots | \, k_n\rangle$ must respect the permutation symmetry acting on the n momenta. In the n-particle Fock space, the completeness relation becomes:

$$(\mathbb{1})_{n \text{ particle}} \;= \frac{1}{n!}\int \frac{d^3k_1}{(2\pi)^3 2k_1^0}\cdots\frac{d^3k_n}{(2\pi)^3 2k_n^0}\,|k_1,\ldots,k_n\rangle\,\langle k_1,\ldots,k_n|$$

Where the $\frac{1}{n!}$ compensates for overcounting of states. The normalization is:

$$\left\langle k_1, \ldots, k_n | k_1', \ldots, k_n' \right\rangle = n! \text{ terms}$$

e.g:

$$\left\langle k_1 k_2 \mid k_1' k_2' \right\rangle = \left((2\pi)^3 2k_1^0 (2\pi)^3 2k_2^0\right) \times \left[\delta^3\left(\vec{k}_1 - \vec{k}_1'\right)\delta^3\left(\vec{k}_2 - \vec{k}_2'\right) + \delta^3\left(\vec{k}_1 - \vec{k}_2'\right)\delta^3\left(\vec{k}_2 - \vec{k}_1'\right)\right]$$

(In effect, we normalize states with coincident momenta differently than those with distinct momenta; the difference is compensated by the $(1/n!)$ in the sum over states.)

The many-particle states transform as the (reducible) representation of the Poincaré group:

$$\begin{aligned} U(\Lambda, a)\,|k_1,\ldots,k_n\rangle &= U(a)U(\Lambda)\,|k_1,\ldots k_n\rangle \\ &= e^{i\Lambda(k_1+k_n)\cdot a}\,|\Lambda k_1,\ldots,\Lambda k_n\rangle \end{aligned}$$

(Eg. $(k_1 + k_2)^2$ is Poincare invariant). The full Hilbert space is a direct sum:

$$\mathcal{H} = \mathcal{H}^{(0)} \otimes \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)} \otimes \ldots \tag{2.1}$$

where $\mathcal{H}^{(0)}$is the zero-particle Hilbert space, $\mathcal{H}^{(1)}$ is the 1-particle Hilbert space, $\mathcal{H}^{(2)}$ is the 2-particle Hilbert space etc.

This (separable) Hilbert space is called Fock space.

Fields

Now we have the complete Hilbert space of the theory, and a representation of the Poincaré group acting on the space. Have we therefore completed the construction? No. This theory, so far, lacks *local* observables – operators with compact support in spacetime. Such observables are called *fields*. A field, technically, is an "operator valued distribution" –if $\phi(x)$ is a field, then

$$\int d^4x\phi(x)f(x)$$

is an operator $\mathcal{H} \to \mathcal{H}$, where f is a suitably smooth test function. The idea of field theory is that quantities that can be measured by an observer localized in spacetime can be modeled as functions of the so-called "smeared" fields.

Observers can communicate by emitting and absorbing particles, so the fields should be able to create or destroy particles– as operators; they mix up the different n-particle spaces $\mathcal{H}^{(n)}$.

A further motivation for introducing fields comes from considering interactions among particles. In a consistent theory, particle interactions are typically local in spacetime and admit a natural description in the language of fields.

We will construct a fundamental field of the theory from which all low-level observables can be constructed. The field $\phi(x)$ is to be regardsd as a Heisenberg operator in the theory.(Since fields depend on x, it is natural that they also depend on t, in a relativistic theory.)

We demand that $\phi(x)$ has the following properties:

(i) ϕ creates or destroys one particle. Then, operators that create or destroy many particles are obtained from polynomials in ϕ.

(ii) $\phi = \phi^\dagger$. We want ϕ to be hermitian so that it will be an observable.

(iii) $U(\Lambda, a)\phi(x)U(\Lambda, a)^{-1} = \phi(\Lambda x + a)$. ϕ transforms as a *scalar* under Poincaré transformations. It is convenient to formulate a relativistic theory in terms of fields that transform as simply as possible.

These conditions suffice to almost completely fiz $\phi(x)$.

To construct $\phi(x)$, it is helpful to first define operators with moentum space arguments that create and destroy particles. Define an operator $A(k)^\dagger$ as follows:

$$A(k)^\dagger : \mathcal{H}^{(0)} \rightarrow \mathcal{H}^{(1)}$$
$$A(k)^\dagger|0\rangle = |k\rangle$$

Similarly, define the action of $A(k)^\dagger$ on $\mathcal{H}^{(n)}$ by:

$$A(k)^\dagger \left|k_1, \ldots, k_n\right\rangle = \left|k, k_1, k_2, \ldots, k_n\right\rangle .$$

This determines all matrix elements of $A(k)^\dagger$ between states in the Fock space $\mathcal{H}$, and hence also determines all matrix elements of its adjoint $A(k)$. For example:

$$\left\langle 0 \left| A(k)^\dagger \right| \text{ arbitrary state} \right\rangle = 0 \Rightarrow A(k)|0\rangle = 0$$
$$\left\langle k' \left| A(k)^\dagger \right| 0 \right\rangle = \langle k'|k\rangle = (2\pi)^3 \left(2k^0\right) \delta^3 \left(\vec{k} - \vec{k}'\right)$$
$$\Rightarrow A(k) \left|k'\right\rangle = (2\pi)^3 \left(2k^0\right) \delta^3 \left(\vec{k} - \vec{k}'\right) |0\rangle.$$

Note that

$$\langle 0 \left[A(k), A\left(k'\right)^+\right] |0\rangle = \left\langle k \mid k'\right\rangle = (2\pi)^3 2k^0 \delta^3 \left(\vec{k} - \vec{k}'\right) \langle 0|0\rangle$$

and one can check that

$$\langle \text{state'} \left[A(k), A\left(k'\right)^+\right] |\text{state}\rangle = (2\pi)^3 2k^0 \delta^3 \left(\vec{k} - \vec{k}'\right) \langle \text{state'}|\text{state}\rangle$$

for arbitrary Fock space basis states. So

$$\left[A(k), A\left(k'\right)^+\right] | = (2\pi)^3 2k^0 \delta^3 \left(\vec{k} - \vec{k}'\right)$$

is an operator identity on Fock space. Note also that

$$|k_1, \ldots, k_n\rangle = A(k_1)^\dagger \ldots A(k_n)^\dagger|0\rangle$$

Thus, the assumed Bose symmetry of the many-particle states implies

$$\left[A(k)^\dagger, A\left(k'\right)^\dagger\right] = 0$$

and hence

$$\left[A(k), A\left(k'\right)\right] = 0.$$

How do the $A(k)$ transform under Poincaré transformations? Using Poincaré invariance of the vacuum:

$$U(a)|k\rangle = e^{ik\cdot a}|k\rangle = U(a)A(k)^\dagger U(a)^{-1}U(a)|0\rangle$$
$$= U(a)A(k)^\dagger U(a)^{-1}|0\rangle = e^{ik\cdot a}A(k)^\dagger|0\rangle$$

So,

$$U(a)A(k)^\dagger U(a)^{-1} = e^{ik\cdot a}A(k)^\dagger$$

acting on the vacuum, and similarly acting on any state. Take adjoints:

$$U(a)A(k)U(a)^{-1} = e^{-ik\cdot a}A(k)$$

$$\begin{aligned}
&U(\Lambda)|k\rangle = |\Lambda k\rangle, \text{ or} \\
&U(\Lambda)A(k)^\dagger U(\Lambda)^{-1}|0\rangle = A(\Lambda k)^\dagger|0\rangle \\
&\Rightarrow \quad U(\Lambda)A(k)^\dagger U(\Lambda)^{-1} = A(\Lambda k)^\dagger \\
&U(\Lambda)A(k)U(\Lambda)^{-1} = A(\Lambda k)
\end{aligned}$$

Now, the most general operator that creates and destroys a one-particle state is a linear combination of A's and $A^\dagger$'s:

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3 2k^0}\left[C(k,x)A(k) + C(k,x)^* A(k)^\dagger\right]$$

It transforms under Lorentz transformations as

$$U(\Lambda)\phi(x)U(\Lambda)^{-1} = \int \frac{d^3k}{(2\pi)^3 2k^0}\left[C(k,x)A(\Lambda k) + C(k,x)^* A(\Lambda k)^\dagger\right]$$

Using Lorentz invariance of measure, we have

$$= \int \frac{d^3k}{(2\pi)^3 2k^0}\left[C\left(\Lambda^{-1}k,x\right)A(k) + C\left(\Lambda^{-1}k,x\right)^* A(k)^\dagger\right]$$

And we require

$$\phi(\Lambda x) = \int \frac{d^3k}{(2\pi)^3 2k^0}\left[C(k,\Lambda x)A(k) + C(k,\Lambda x)^* A(k)^\dagger\right]$$

Therefore, $C(k,x)$ must be a Lorentz invariant function:

$$C\left(\Lambda^{-1}k,x\right) = C(k,\Lambda x) \text{ or } (1\Lambda k,\Lambda x) = C(k,x)$$

C is a function of the Lorentz-invariant variables $m^2 = k^2, x^2, k\cdot x$.
Now, under translations,

$$U(a)\phi(x)U(a)^{-1} = \int \frac{d^3k}{(2\pi)^3 2k^0}\left[C(k,x)e^{-ik\cdot a}A(k) + C(k,x)^* e^{ik\cdot a}A(k)^\dagger\right]$$

This implies

$$\phi(x+a) = \int \frac{d^3k}{(2\pi)^3 2k^0} \left[C(k, x+a) A(k) + C(k, x+a)^* A(k)^\dagger \right]$$

So C must satisfy

$$C(k, x+a) = e^{-ik\cdot a} C(k, x)$$

This determines the x dependence up to a multiplicative constant:

$$C(k, x) = c = Ce^{-ik\cdot x}$$

In fact, the phase of C is unphysical. We can absorb the phase by adjusting the phase of $A(k)$, or equivalently, by adopting a different phase convention for the states $|k\rangle$. Therefore, we can take C to be real and

$$\phi(x) = C \int \frac{d^3k}{(2\pi)^3 2k^0} \left[e^{-ik\cdot x} A(k) + e^{ik\cdot x} A(k)^\dagger \right]$$

So we have determined ϕ up to a real normalization constant. This constant quantifies the amplitude for ϕ to create a one-particle state:

$$\langle k|\phi(x)|0\rangle = Ce^{ik\cdot x}$$

We can choose C=1 by convention.

The states $\phi(x)|0\rangle$ provide a basis for $\mathcal{H}^{(1)}$ that is in a sense conjugate to the plane wave basis. Note that this is a complete basis. And the states

$$\phi(x_1) \ldots \phi(x_n) |0\rangle$$

form a complete basis for the n-particle space $\mathcal{H}^{(n)}$. Thus, polynomials in the fields, acting on the vacuum, span the Fock space. We say, in this case, that the fields are a *complete* set of local observables.

Causality

Now we have a relativistic field theory with local observables, but there is one more thing to check – that the theory satisfies relativistic *causality.*

Causality requires that if measurements are performed in regions 1 and 2 shown in Fig5, that have spacelike separation, the measurements in 1 should not affect the outcome of measurements in region 2 and vice versa. In quantum mechanics, this means that observables measured in regions 1 and 2 must *commute*:

$$0 = [\theta(1), \theta(2)]$$

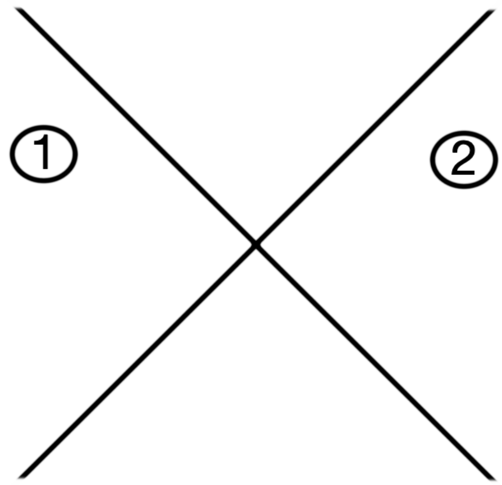

Figure 1. Regions 1 and 2 are spacelike separated

where regions 1 and 2 are spacelike separated.

If all observables can be constructed from smeared fields, then it is necessary (and sufficient) that

$$[\phi(x), \phi(y)] = 0, \quad (x-y)^2 < 0.$$

Is this true? Yes, and for a subtle reason.

Let's decompose $\phi(x)$ into a piece that annihilates particles and a piece that creates particles:

$$\begin{aligned}
\phi(x) &= \phi^{(-)} + \phi^{(+)} \\
\phi^{(-)} &= \int \frac{d^3k}{(2\pi)^3 2k^0} e^{-ik\cdot x} A(k) \\
\phi^{(+)} &= \int \frac{d^3k}{(2\pi)^3 2k^0} e^{ik\cdot x} A(k)^\dagger
\end{aligned}$$

Consider the function

$$\begin{aligned}
&G(x-y) = [\phi(x), \phi(y)] = \langle 0|\phi^{(-)}(x)\phi^{(+)}(y)|0\rangle \\
&= \int \frac{d^3k}{(2\pi)^3 2k^0} e^{-ik\cdot(x-y)}
\end{aligned}$$

Note that, because of the Lorentz invariance of the measure, G_+ is a Lorentz-invariant function

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

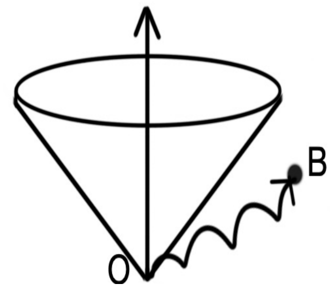

Figure 2. Propagation outside lightcone. OB is a spacelike interval.

. We could evaluate this integral (and express G_+ in terms of a modified Bessel function), but even without explicitly evaluating it, we can see that $G_+(x)$ does *not* have the property of vanishing for spacelike x. The reason is that G_+ is an analytic function and cannot vanish in an open set without vanishing throughout its domain of analyticity.

G_+ is analytic because of the positivity condition on the energy of a particle, $k^0 > 0$. If we express

$$G_+(x) = \int \frac{d^4k}{(2\pi)^3} \theta\left(k^0\right) \delta\left(k^2 - m^2\right) e^{-ik\cdot x}$$

we can see that G_+ is a sum of entire functions $e^{-ik\cdot x}$, and because k^0 is restricted to be positive, this sum converges for $\operatorname{Im} x^0 < 0$ – it is damped by the exponential. So real x^0 is at the very least on the boundary of the domain of analyticity. In fact, G_+ does decay like $exp[-m|x^2|^{\frac{1}{2}}]$ for x outside the light cone, but it is not zero.

This sounds like a serious breach of causality – since $G_+(x) = \langle 0 \left| \phi^{(-)}(x)\phi^{(+)}(0) \right| 0\rangle \neq 0$ for x spacelike, the particle excitations localized at x seems to propagate outside the light cone, just as we feared. But can this propagation really be detected?

Let's consider a commutator of *observables*:

$$\begin{aligned} iG(x-y) = [\phi(x), \phi(y)] &= \left[\phi^{(-)}(x), \phi^{(+)}(y)\right] + \left[\phi^{(+)}(x), \phi^{(-)}(y)\right] \\ &= G_+(x-y) - G_+(y-x) \end{aligned}$$

But notice that, because $G_+(x)$ is Lorentz-invariant, it must be an even function, $G_+(x) = G_+(-x)$, for spacelike x, there is a proper Lorentz transformation that takes $x^0 \to -x^0$ and $\vec{x} \to -\vec{x}$. (Note that G_+ does not have this property for x timelike. It is not invariant under time reversal because only *positive* k^0 appears). Hence,

$$[\phi(x), \phi(y)] = 0 \quad (x-y)^2 < 0$$

The fields *are* causal observables.

Causality actually results fromm a remarkable interference effect. There is (in a sense) propagation outside the light cone from x to y, but there is also propagation from y to x. Because the amplitudes for these processes interfere *destructively*, measurements at x and y do not influence one another.

Remarks:

- If we had considered a theory of particles that carry the value Q of a conserved charge, then the propagation of a particle with charge -Q would be necessary to destructively interfere with the propagation of a charge Q particle outside the light cone. Together, causality and the positivity of the energy require, in a relativistic theory, the existence of *antiparticles*.

- Causality severely restricts the algebra of observables in a relativistic theory. With the phase convention that we adopted, we find

$$\phi'(x) = \int \frac{d^3k}{(2\pi)^3 2k^0} \left[e^{-ik\cdot x} A(k) + e^{ik\cdot x} A(k)^\dagger \right].$$

  But had we adopted a different convention, we could have had

$$\phi^\theta(x) = \int \frac{d^3k}{(2\pi)^3 2k^0} \left[e^{-ik\cdot x} e^{-i\theta} A(k) + e^{ik\cdot x} e^{i\theta} A(k)^\dagger \right].$$

  Including both $\phi(x)$ and $\phi^\theta(x)$ as local observables in the theory is worse than redundant because ϕ and ϕ^θ are not local relative to one another unless we have $e^{-i\theta} = 1$. We have $[\phi^\theta(x), \phi(y)] = e^{-i\theta}\Delta_+(x-y) - e^{i\theta}\Delta_+(y-x) = -2i\sin\theta\Delta_+(x-y)$ for $(x-y)^2 < 0$.

So we see that the algebra of observables is an exclusive club - no operator may join unless it commutes, at spacelike separation, with all operators that already belong. In particular, ϕ^θ (for $e^{-i\theta} \neq 1$) cannot be admitted if ϕ is already a member.

Some further properties of the field theory:

Field Equation

Observe that $\phi(x)$ satisfies a covariant wave equation, $\left(\partial^\mu\partial_\mu + m^2\right)\phi(x) = 0$, known as the Klein-Gordon equation. This wave equation is a consequence of the mass shell condition $P^\mu P_\mu = m^2$ satisfied by the particles. The equation has positive-frequency solutions $e^{-ik\cdot x}$ and negative-frequency solutions $e^{ik\cdot x}$, where $k^2 = m^2$.

The negative-frequency solutions caused confusion when $\phi(x)$ was interpreted as a single-particle *wave function*. But we' have seen that they have a simple and natural interpretation if ϕ is an *operator* that creates and destroys particles.

4-Momentum Operator:

The 4-momentum P^μ satisfying $P^\mu|k\rangle = k^\mu|K\rangle$ can be expressed in terms of A and $A^\dagger$. It is given by

$$P^\mu = \int \frac{d^3k}{(2\pi)^3 2k^0} k^\mu A(k)^\dagger A(k).$$

The properties $P^\mu|0\rangle = 0$ and $[P^\mu, A(k)] = -k^\mu A(k)$ (which follows from $e^{iP\cdot a}A(k)e^{-iP\cdot a} = e^{-ik\cdot a}A(k)$) are easily verified.

Conventional Normalization:

Although it is obviously convenient to expand

$$\phi = \int \frac{d^3k}{(2\pi)^3 2k^0} \left[e^{-ik\cdot x}A(k) + e^{ik\cdot x}A(k)^\dagger\right]$$

in terms of creation and annihilation operators for relativistically normalized states, it is more conventional to introduce

$$a(k) = \frac{A(k)}{(2\pi)^{3/2}(2k^0)^{1/2}}$$

so that

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

Then we have

$$\phi(x) = \int \frac{d^3k}{(2\pi)^{3/2}(2k^0)^{1/2}}[e^{-ik\cdot x}a(k) + e^{ik\cdot x}a(k)^\dagger].$$

Alternative Construction of Hilbert Space

The construction of the one-particle Hilbert space $\mathcal{H}^1$ can be described in alternative language, which is not needed now but will prove useful when we consider the theory of fields on a curved background.

Note first that when a local field is constructed, the overlap of an arbitrary state with $\phi(x)|0\rangle$, for all x, provides a natural $1-1$ map:

$$\mathcal{H}^{(1)} \simeq \{\textit{positive} \text{ frequency solutions to the Klein-Gordon equation}\}$$

The state

$$|\tilde{f}\rangle = \int \frac{d^3x}{(2\pi)^3 2k^0}\tilde{f}(k)|k\rangle$$

is associated with the solution

$$\langle 0|\phi(x)|k\rangle = \int \frac{d^3k}{(2\pi)^3 2k^0}\tilde{f}(k)e^{-ik\cdot x}$$

Equivalently,

$$\langle 0|\phi(x)|k\rangle^* = \langle k|\phi(x)|0\rangle$$

provides the $1-1$ map.

$$\mathcal{H}^{(1)} \simeq \left\{\textit{negative} \text{ frequency solutions to K.G. equation}\right\}$$

This observation can also serve as the starting point of the construction of the scalar quantum field theory. The classical field theory is defined by the classical Klein-Gordon field equation

$$\left(\partial^\mu \partial_\mu + m^2\right)\phi(x) = 0$$

To obtain a quantum theory, we begin by constructing the "one particle" Hilbert space $\mathcal{H}^{(1)}$. The general solution to the K-G. equation can be expanded in the basis

$$\begin{aligned} u_k(x) &= e^{-ik\cdot x} \quad \text{- positive frequency} \\ u_k(x)^* &= e^{ik\cdot x} \quad \text{- negative frequency.} \end{aligned}$$

If Lorentz transformations act on the solutions according to

$$\Lambda : f(x) \to f\left(\Lambda^{-1}x\right)$$

(Note: the *opposite* of how the quantum field ϕ transforms), then the positive frequency and negative frequency basis each transform irreducibly under the proper Lorentz transformations:

$$\begin{aligned} \Lambda &: u_k(x) \to u_k\left(\Lambda^{-1}x\right) = u_{\Lambda k}(x) \\ \Lambda &: u_k(x)^* \to u_k\left(\Lambda^{-1}x\right)^* = u_{\Lambda k}(x)^* \end{aligned}$$

The proper Lorentz transformations do not mix up positive and negative frequency, so the positive (or negative) frequency solutions are a linear space on which Lorentz transformations act irreducibly(and translations, too.)

Solutions of the K.G. equation are also in one-to-one correspondence with initial value data: the solution to $\left(\partial^\mu \partial_\mu + m^2\right) f(x) = 0$ is uniquely determined by values of f and $\dot{f}$ on a surface $x^0 = t =$ constant. But for a solution of definite frequency (e.g. positive), the $\dot{f}$ initial data is not necessary to propagate f from the initial-value surface. There are $1-1$ correspondences:

$$\{\text{ positive frequency solutions }\} \simeq \{\text{ negative frequency solutions }\} \simeq \left\{\text{ functions on } \mathbb{R}^3\right\}.$$

To obtain a Hilbert space, we must specify an inner product. To define the inner product of two solutions, specify a time t and integrate over the time slice:

$$(f,g) = i\int_t d^3x\, [f^*(x)\partial_t g(x) - \partial_t f^*(x) g(x)]$$

(Note: Birrell and Davies define $(f,g)^*$ as above.)

Then, for the basis $u_k(x) = e^{-ik\cdot x}$, we have

$$\begin{aligned}
(u_k, u_{k'}) &= (2\pi)^3 2k^0 \delta^3(\vec{k} - \vec{k'}) \\
(u_k, u^*_{k'}) &= 0 \\
(u^*_{k'}, u_k) &= -(2\pi)^3 2k^0 \delta^3(\vec{k} - \vec{k'})
\end{aligned}$$

This Klein-Gordon inner product is not positive definite on the space of all solutions. But it is positive definite on the space of positive frequency solutions. Furthermore, (f,g) is positive definite for negative frequency solutions, and the positive and negative frequency solutions are orthogonal to each other. There is a natural decomposition of the space of all solutions:

$$\{\text{solutions}\} = \{\text{positive frequency}\} \oplus \{\text{negative frequency}\},$$

such that the direct sum is a sum of spaces that are *orthogonal* with respect to the Klein-Gordon inner product.

The basis $u_k(x)$ for the positive frequency solutions has precisely the normalization as in the plane wave basis for $\mathcal{H}^{(1)}$:

$$\langle k|k'\rangle = (2\pi)^3 2k^0 \delta^3(\vec{k} - \vec{k'}),$$

so the $u_k(x)$'s correspond to relativistically normalized one-particle plane wave states.

In defining (f,g), we seem to have picked out a particular frame and a particular slice. But we can rewrite (f,g) in a form that is manifestly invariant under deformations of the spacelike surface. We write:

$$(f,g) = i\int_\Sigma d^3x\, n^\mu \left[f^*\partial_\mu g - \partial_\mu f^* g\right],$$

where we integrate over a spacelike 3-dimensional hypersurface Σ, and n^μ is the normalized unit (timelike) normal to Σ in the forward light cone.

If we distort the surface Σ_1 to a new surface Σ_2, we get:

$$\begin{aligned}
(f,g)_{\Sigma_1} - (f,g)_{\Sigma_2} &= i\int_{\Sigma_1 - \Sigma_2} d^3x\, n^\mu \left(f^*\partial_\mu g - \partial_\mu f^* g\right) \\
&= i\int_\Omega d^4x\, \partial^\mu \left(f^*\partial_\mu g - \partial_\mu f^* g\right), \text{ where } \partial\Omega = \Sigma_1 - \Sigma_2
\end{aligned}$$

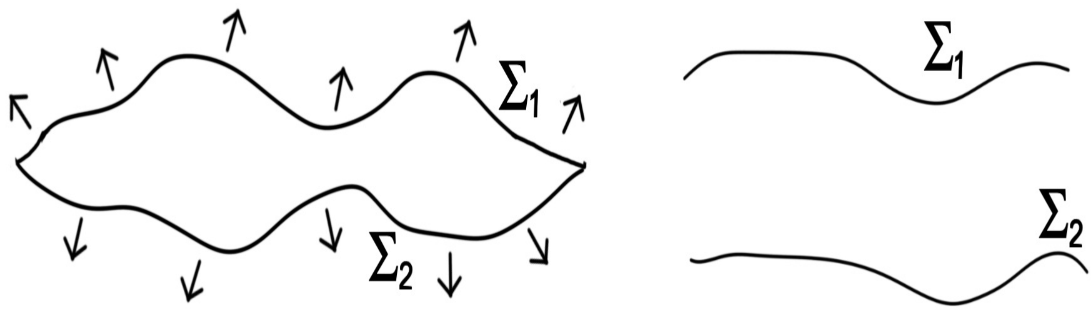

Figure 3. Left: Two hyper surfaces $\Sigma_1, Sigma_2$ that can be distorted into one another. Right: Two hypersurfaces for which $\Sigma_1 - \Sigma_2$ is not a closed surface.

(using the divergence theorem). But since both f and g are solutions to the Klein-Gordon equation:

$$\begin{aligned} \partial^\mu \left(f^* \partial_\mu g - \partial_\mu f^* g\right) &= f^* \partial^2 g - \partial^2 f^* g \\ &= (m^2 - m^2) f^* g = 0 \end{aligned}$$

So, $(f,g)_{\Sigma_1} - (f,g)_{\Sigma_2} = 0$. This conclusion holds even if $\Sigma_1 - \Sigma_2$ is not a closed surface or if Σ_1 and Σ_2 are infinite spacelike slices, and there is no contribution to the integral from spatial infinity (which is true for normalized states).

We have now described how, beginning with the classical field equation, we can construct $\mathcal{H}^{(1)}$ as a sum of positive frequency solutions. Once we have $\mathcal{H}^{(1)}$, we can obtain $\mathcal{H}^{(n)}$ as a symmetrized tensor product, e.g.:

$$\mathcal{H}^{(2)} = \mathcal{H}^{(1)} \otimes_s \mathcal{H}^{(1)}.$$

Then we proceed to construct $A(k)$ and $\phi(x)$ as before, obtaining:

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3 2k^0} \left[u_k(x) A(k) + u_k(x)^* A(k)^\dagger\right].$$

Relation to canonical methods

Recall that:

$$[\phi(x), \phi(y)] = G_+(x-y) - G_+(y-x)$$

and therefore

$$[\phi(x), \dot{\phi}(y)] = \int \frac{d^3k}{(2\pi)^3 k^0} \left[ik^0 e^{-ik\cdot(x-y)} + ik^0 e^{ik\cdot(x-y)}\right]$$
$$[\dot{\phi}(x), \dot{\phi}(y)] = \int \frac{d^3k}{(2\pi)^3 k^0} (k^0)^2 \left[e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)}\right]$$

If we evaluate these at equal times $x^0 - y^0 = 0$, we find:

$$[\phi(x), \phi(y)]_{\text{et}} = 0$$
$$[\phi(x), \dot{\phi}(y)]_{\text{et}} = i\delta^3(\vec{x} - \vec{y})$$
$$[\dot{\phi}(x), \dot{\phi}(y)]_{\text{et}} = 0$$

Since $G_+(x)$ is a Lorentz-invariant function, these identities hold in all inertial reference frames. They recall the commutation relations:

$$[q_i, q_j] = 0$$
$$[q_i, p_j] = i\delta_{ij}$$
$$[p_i, p_j] = 0$$

of a canonical quantum mechanical system (with $\hbar = 1$), except with continuum normalization. (The continuum normalization reminds us that the fields are *distributions*. We could obtain the discrete normalization by smearing the fields with some complete set of square-integrable functions.)

These canonical commutation relations are equivalent to the commutation relations satisfied by the $A(k)$'s and $A(k)^\dagger$'s. If we Fourier transform, we have:

$$\tilde{\phi}(t, \vec{k}) = \int d^3\vec{x} e^{-i\vec{k}\cdot\vec{x}} \phi(t, \vec{x})$$
$$\tilde{\phi}(t, \vec{k})^\dagger = \tilde{\phi}(t, -\vec{k})$$
$$\text{and } [\tilde{\phi}, \tilde{\phi}]_{et} = [\dot{\tilde{\phi}}, \dot{\tilde{\phi}}]_{et} = 0$$

$$\left[\tilde{\phi}(t, \vec{k}), \dot{\tilde{\phi}}\left(t, -\vec{k}'\right)\right] = i(2\pi)^3 \delta^3\left(\vec{k} - \vec{k}'\right)$$

where

$$\tilde{\phi}(t, \vec{k}) = \frac{1}{2k^0}\left[e^{-ik^0 t} A\left(k^0, \vec{k}\right) + e^{ik^0 t} A\left(k_0, -\vec{k}\right)^\dagger\right]$$
$$\dot{\tilde{\phi}}(t, \vec{k}) = -\frac{i}{2}\left[e^{-ik^0 t} A\left(k^0, \vec{k}\right) - e^{ik^0 t} A\left(k_0, -\vec{k}\right)^\dagger\right]$$

and hence

$$\text{adjoint } \Rightarrow e^{-ik^0t}A(k) = k^0\tilde{\phi}(t,-\vec{k}) + i\dot{\tilde{\phi}}(t,-\vec{k})$$
$$\text{adjoint } \Rightarrow e^{ik^0t}A(k)^\dagger = k^0\tilde{\phi}(t,-\vec{k}) - i\dot{\tilde{\phi}}(t,-\vec{k})$$

So the commutation relations

$$\left(A(k), A\left(k'\right)\right] = 0 = \left[A(k)^\dagger, A\left(k'\right)^\dagger\right].$$
$$\left[A(k), A\left(k'\right)^\dagger\right] = (2\pi)^3 2k^0\delta^3\left(\vec{k}-\vec{k}'\right)$$

can evidently be recovered from the equal time commutators of ϕ and $\dot{\phi}$ as well as vice versa.

To complete the specification of the canonical system, we need a Hamiltonian H expressed in terms of ϕ and its conjugate momentum $\pi = \dot{\phi}$. H is thus P^0, the generator of time evolutions satisfying

$$\left[P^0, A(k)\right] = -k^0A(k)$$
$$\left[P^0, A(k)^\dagger\right] = k^0A(k)^\dagger$$

and therefore

$$[H, \phi(x)] = -i\dot{\phi}(x)$$
$$[H, \pi(x)] = -i\dot{\pi}(x)$$

We have

$$H = \int \frac{d^3k}{(2\pi)^3 2k^0} k^0 A(k)tA(k)$$

where

$$A(k)^+A(k) = \tilde{\pi}(t,\vec{k})\tilde{\pi}(t,-\vec{k}) + \left(k^0\right)^2\tilde{\phi}(t,\vec{k})\tilde{\phi}(t,-\vec{k}) + ik^0[\tilde{\phi}(t,-\vec{k})\tilde{\pi}(t,\vec{k}) - \tilde{\pi}(t,-\vec{k})\tilde{\phi}(t,\vec{k})]$$
$$\text{So } H = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2}\left[\tilde{\pi}(t,\vec{k})\tilde{\pi}(t,-\vec{k}) + \left(k^0\right)^2\tilde{\phi}(t,\vec{k})\tilde{\phi}(t,-\vec{k}) - k^0(2\pi)^3\delta^3(0)\right]$$

Up to an additive constant, this is the Hamiltonian of an infinite set of uncoupled harmonic oscillators, where the oscillator labeled $\vec{k}$ has frequency $\omega_k = k^0 = \sqrt{\vec{k}^2 + m^2}$.

To understand the origin of the constant, note that $(2\pi)^3\delta^3(0) = \int d^3x(1) = V$ is the spatial volume, and $d^3k/(2\pi)^3$ is the density of oscillator modes per unit volume,

$$H_0 = \text{ constant } = -\sum_{\text{modes}}\left(\frac{1}{2}\omega_k\right)$$

The constant subtracts away the zero-point energy of all the oscillators. We make this subtraction so that $P^\mu|0\rangle = 0$.

Otherwise, we normally aim to split P^μ up into two pieces, where one piece transforms as a four-vector, and the remainder, $\langle 0|P^\mu|0\rangle$, is invariant under Lorentz transformations.

Canonical Quantization

The canonically quantized theory can be arrived at starting from a classical theory defined by an action principle.

To define a relativistic scalar field theory, we may specify that $\phi(x)$ is a scalar field

$$(\Lambda, a) : \phi(x) \to \phi(\Lambda x + a)$$

and construct

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

We require:

- S is local and a functional of ϕ and first derivatives, so that the initial value problem is well formulated.
- $\mathcal{L}$ is Poincaré invariant (frame independent dynamics).
- $\mathcal{L}$ is quadratic in ϕ and $\partial^\mu \phi$(linear equation oof motion, free field theory).

The Lagrangian density is:

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

This is unique (for $m^2 \neq 0$) – up to a linear redefinition of ϕ. We remove any term linear in ϕ by $\phi \to \phi + b$ and (remove call the first term by $\phi \to c\phi$). Positivity of energy will require $m^2 \geq 0$ and positive coefficient of the $\frac{1}{2}\partial^\mu \phi \partial_\mu \phi$ term. For $m^2 = 0$, no linear term is allowed.

We obtain field equations from the action principle:

$$0 = \delta S = \int d^4x \left[\frac{\partial \mathcal{L}}{\partial \phi}\delta\phi + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi}\delta \partial_\mu \phi\right] = \int d^4x \delta\phi \left[\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi}\right] + \text{ surface term}$$

$$\Rightarrow \frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} = 0 \text{ (if } \delta S = 0 \text{ for arbitrary variations that vanish at the boundary.)}$$

For the above $\mathcal{L}$, we have $\left(\partial_\mu \partial^\mu + m^2\right)\phi(x) = 0$ - the Klein-Gordon equation.

We construct the canonical Hamiltonian $H = \sum_i \dot{q}_i p_i - L, \quad p_i = \frac{\partial L}{\partial \dot{q}_i}$:

$$H = \int d^3x (\dot{\phi}\pi - \mathcal{L}), \quad \pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}}$$

where $\dot{\phi}$ is eliminated in favor of π.

For the free scalar field theory, we have:

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

We obtain a quantum field theory by requiring that ϕ and π obey canonical commutation relations at equal times (they are to be regarded as Heisenberg operators):

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

The $\phi(t, \vec{x})$ at fixed t may be regarded as a complete set of commuting observables for the canonical system.

If we expand ϕ and $\dot{\phi} = \pi$ in terms of A and $A^\dagger$, we obtain again the quantum theory discussed previously. We chose a particular frame in which to canonically quantize, but the commutation relations are the same in all inertial frames, which is crucial to ensure that the theory is causal(ϕs commute at spacelike separation).

Since the theory is Poincaré invariant, we can construct conserved quantities by the Noether procedure. For instance, from translational invariance, we obtain:

$$\partial_\nu T^{\mu\nu} = 0, \text{ where } T^{\mu\nu} = \partial^\mu \phi \partial^\nu \phi - \eta^{\mu\nu} \mathcal{L}$$

is the canonical energy-momentum tensor. We will not derive this here, as we will soon obtain $T^{\mu\nu}$ by another method.

The conserved four-momenta are then:

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

There is an ordering ambiguity in $P^0 = H$, which, as we noted before, can be resolved by demanding $\langle 0 | P^\mu | 0 \rangle = 0$. The corresponding ordering prescription is called *normal* ordering.

- Canonical quantization is a noncovariant procedure. We must choose a frame to define a Hamiltonian H. But we have seen that the theory that we obtain *is* covariant(admits a unitary representation of the Poincaré group).

- The canonical quantization method gives a quantum theory that agrees with a given classical theory in the classical limit. (Hamilton's equations are satisfied at the operator level:

$$\dot{q} = -i[q, H] = \frac{\partial H}{\partial p} \left(\because q \sim i\frac{\partial}{\partial p} \right)$$
$$\dot{p} = -i[p, H] = -\frac{\partial H}{\partial q}$$

  Thus, it is natural tp apply this procedure to obtain a quantum version of a field that is observable classically – e.g., the electromagnetic field. Canonical quantization is much less natural if we are trying to devise a relativistic theory of pions or electrons).

- Canonical quantization has an important advantage over other procedures - it is easily applied to an interacting (nonlinear) theory. Our construction of the Klein-Gordon inner product required that the field equation be linear(in order to be slice independent) and our Fock space construction assumed that the particles are non-interacting.

3 Field Theory in Curved Space-Time

Our experience with field theory on flat spacetime has prepared us to confront the problem of constructing quantum fields on a curved background.

The idea is the idea that we always invoke to promote flat-spacetime physics to more general covariant physics. Locally (at sufficiently short distances), spacetime is approximately flat. Our field theory on curved spacetime should reduce to flat-spacetime physics locally. Because we must consider local physics, it is essential that we describe quantum field theory in terms of local field variables.

If our flat spacetime theory is causal, then so will the theory on curved spacetime be causal - if it reduces to a flat theory locally. If information does not propagate outside the light cone *locally*, then it stays within the light cone *globally*.

The concept of a particle, which was fundamental in our discussion on flat spacetime, is less essential in the formulation of field theory on a curved background. A particle, as we defined it, is an IR of the Poincaré group. But a curved background will not be Poincaré invariant, nor will the quantum field built on it admit a unitary representation of the Poincaré group. The notion of a particle is an approximate one, valid when the wavelength is much smaller than the length scale characteristic of curvature. (In practice, this limitation the need not be serious. For example, the width of the Z^0 is not very sensitive to the Hubble constant H_0.)

Classical Scalar Field on Curved Spacetime

To begin, we construct the Klein-Gordon classical field theory on a nontrivial background. The flat spacetime action

$$S = \int d^4x \, \frac{1}{2} \left[\eta^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - m^2 \phi^2\right]$$

may be written as

$$S = \int d^4x \sqrt{g} \frac{1}{2} \left[g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - m^2 \phi^2\right]$$

where $g = -\det(g_{\mu\nu})$, so that $d^4x\sqrt{g}$ is the invariant volume element. In this form, S is invariant under local coordinate transformations

$$x \to x'(x)$$

where ϕ is a scalar transforming as

$$\phi(x) \to \phi\left(x'\right)$$

From this action, we derive the Euler-Lagrange equation:

$$
\begin{aligned}
&\partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \\
&\text{where} \quad \mathcal{L} = \sqrt{g}\left(\frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - \frac{1}{2} m^2 \phi^2\right) \\
&\text{or} \quad \frac{1}{\sqrt{g}} \partial_\mu \left(\sqrt{g} g^{\mu\nu} \partial_\nu \phi\right) + m^2 \phi = 0
\end{aligned}
$$

We can put this equation in a more recognizable form by invoking an identity

$$\frac{1}{\sqrt{g}} \partial_\mu \sqrt{g} = \Gamma^\lambda_{\lambda\mu}$$

Thus, we have

$$\partial_\mu \partial^\mu \phi + \Gamma^\lambda_{\lambda\mu} \partial^\mu \phi + m^2 \phi = 0$$

or

$$\boxed{\left(\nabla_\mu \nabla^\mu + m^2\right) \phi = 0} \tag{3.1}$$

where covariant derivatives ∇_μ of a scalar is

$$\nabla_\mu \phi = \partial_\mu \phi$$

and of a 4-vector is

$$\nabla_\mu V^\nu = \partial_\mu V^\nu + \Gamma^\nu_{\mu\lambda} V^\lambda \Rightarrow \nabla_\mu V^\mu = \partial_\mu V^\mu + \Gamma^\lambda_{\lambda\mu} V^\mu$$

is covariant divergence.

The boxed equation is the flat space KG equation, with derivatives replaced by covariant derivatives.

To derive the identity, assume that for any matrix M,

$$
\begin{aligned}
\ln \det(M + \delta M) &= \operatorname{tr} \ln(M + \delta M) \\
&= \operatorname{tr}[\ln M + \ln(\mathbb{1} + M^{-1} \delta M)] \\
&= \operatorname{tr} \ln M + \operatorname{tr} M^{-1} \delta M
\end{aligned}
$$

or

$$
\begin{aligned}
\frac{\delta(\det M)}{\det M} &= \operatorname{tr} M^{-1} \delta M \\
\delta \sqrt{\det M} &= \frac{1}{2} \sqrt{\det M} \operatorname{tr} M^{-1} \delta M
\end{aligned}
$$

thus

$$\delta \sqrt{g} = \frac{1}{2} \sqrt{g} g^{\mu\nu} \delta g_{\mu\nu}.$$

Therefore,

$$\frac{1}{\sqrt{g}}\partial_\mu\sqrt{g} = \frac{1}{2}g^{\lambda\nu}\partial_\mu g_{\lambda\nu}$$

. Recalling

$$\Gamma^\lambda_{\mu\nu} = \frac{1}{2}g^{\lambda\sigma}[\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}]$$
$$\Rightarrow \Gamma^\lambda_{\lambda\nu} = \frac{1}{2}g^{\lambda\sigma}[\partial_\lambda g_{\nu\sigma} + \partial_\nu g_{\lambda\sigma} - \partial_\sigma g_{\lambda\nu}]$$
$$= \frac{1}{2}g^{\lambda\sigma}\partial_\nu g\lambda\sigma \text{ (first and third terms cancel)}$$

we have $\frac{1}{\sqrt{g}}\partial_\mu\sqrt{g} = \Gamma^\lambda_{\lambda\mu}$.

It is convenient to formulate the field theory in terms of an action principle because then we can easily extract the stress tensor that acts on a source in the Einstein equation.

If the action for gravity coupled with matter is

$$S = S_{\text{grav}} + S_{\text{matter}}$$

where

$$S_{\text{grav}} = \frac{-1}{16\pi G}\int d^4x\sqrt{g}R$$

and we vary the metric

$$g_{\mu\nu} \to g_{\mu\nu} + \delta g_{\mu\nu},$$

Then

$$\delta S_{\text{grav}} = \frac{-1}{16\pi G}\int d^4x\sqrt{g}G^{\mu\nu}\delta g_{\mu\nu}$$

, where

$$G^{\mu\nu} = R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R.$$

We can now define a stress tensor by

$$\delta S_{\text{matter}} = -\frac{1}{2}\int d^4x\sqrt{g}T^{\mu\nu}\delta g_{\mu\nu}$$

then the equation of motion is

$$G^{\mu\nu} = -8\pi G T^{\mu\nu}$$

- the Einstein equation. To derive $T^{\mu\nu}$ from

$$S = \int d^4x\sqrt{g}\frac{1}{2}\left[g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - m^2\phi^2\right],$$

we use

$$\delta\sqrt{g} = \frac{1}{2}\sqrt{g}g^{\mu\nu}\delta g_{\mu\nu}$$

and

$$\delta g^{\sigma\lambda} = -g^{\mu\nu}g^{\lambda\sigma}\delta g_{\mu\nu}$$

which follows from $\delta\mathcal{M}^{-1} = -M^{-1}\delta M M'$.

Thus

$$T^{\mu\nu} = \partial^\mu\phi\partial^\nu\phi - \frac{1}{2}g^{\mu\nu}\left[g^{\lambda\sigma}\partial_\lambda\phi\partial_\sigma\phi - m^2\phi^2\right]$$

Note: Coordinate invariance of $S_{\text{matter}} \Rightarrow \nabla_\nu T^{\mu\nu} = 0]$.

Quantization in Curved Spacetime

Now we want to construct a Hilbert space such that the fields acting on this space are consistent. To do this, we will use one of the *solutions* to the classic KG equation, on which a natural "inner product" can be defined.

Let f, g be solutions to

$$\left(\nabla_\mu\nabla^\mu + m^2\right)f(x) = 0$$

The Klein-Gordon "inner product" of two solutions is defined by choosing a spacelike surface Σ, and integrating -

$$(f,g) = i\int_\Sigma d^3x\sqrt{h}n^\mu\left[f^*\partial_\mu g - (\partial_\mu f^*)\,g\right]$$

where h_{ij} is the induced 3-metric on the surface Σ, and n^μ is the forward-pointing unit normal on Σ. This form has the desirable property of being independent of the slice Σ. This follows from Gauss's theorem, which can be written in the form

$$\int_\mu d^4x\sqrt{g}\nabla^\mu V_\mu = \int_{\partial\mu} d^3x\sqrt{h}n^\mu V_\mu$$

where V_μ is a 4-vector. (Remember that $\nabla^\mu V_\mu = \frac{1}{\sqrt{g}}\partial^\mu\left(\sqrt{g}V_\mu\right)$ and that g reduces to h in an orthonormal coordinate system with $n^\mu = (1,0,0,0)$.)

Hence

$$\begin{aligned}
(f,g)_{\Sigma_1} - (f,g)_{\Sigma_2} &= \int_{\Sigma_1-\Sigma_2} d^3x\sqrt{h}n^\mu\left(f^*\partial_\mu g - \partial_\mu f^* g\right) \\
&= \int_\Omega d^4x\sqrt{g}\nabla^\mu\left(f^*\nabla_\mu g - \nabla_\mu f^* g\right) \quad (\text{where } \partial\Omega = \Sigma_1 - \Sigma_2)) \\
&= 0 \quad (\text{if } f,\, g \text{ solve the Klein-Gordon equation}).
\end{aligned}$$

This is just as in the flat space case.

Remarks

- It is, of course, implicit in this construction that the Klein-Gordon equation has solutions that are globally defined in spacetime. For this purpose, it suffices that the spacetime be "globally hyperbolic" - that is, that it have a *Cauchy surface.*

What is a "Cauchy surface"? It is, first of all, a "closed achronal slice" of the spacetime - a 3-surface Σ (without boundary) such that any two points on Σ are connected by a timelike or null curve. To be Cauchy, Σ must also have the following property:

For every point p in the spacetime, every timelike or null curve through p (without a past or future endpoint) crosses Σ.

The idea is that this definition tells us that the initial data on Σ completely determines the physics in the future and past of Σ. So, in particular, initial data on Σ is sufficient to determine the solution to the Klein-Gordon equation throughout the spacetime.

In fact, it turns out that if the spacetime has one Cauchy surface, then there is a Cauchy surface through every point. Furthermore, we can choose a time coordinate t so that each $t =$ constant surface is Cauchy. (Technically, a "time coordinate" is a scalar function $t(x)$, assumed such that $(\partial_\mu t)\,(\partial^\mu t) > 0$.)

The globally hyperbolic spacetimes, then, share with flat space the property that

$$\begin{aligned} &\{\text{global solutions to the KG equation}\} \\ &\simeq \{\text{initial data on a "time slice" } \Sigma\} \end{aligned}$$

(References:
R. Wald, "General Relativity," chapters 8, 10.
R. Geroch and G. Horowitz, "Global structure of spacetimes" in "General Relativity: An Einstein Centenary Survey," eds. S. W. Hawking and W. Israel, p. 212-293.)

- The existence of a Klein-Gordon inner product that does not depend on the slice Σ. It actually holds more generally than a free field on a curved background; it extends to any coupling to external sources such that the field equation for ϕ is linear and homogeneous (action S is quadratic). For example, it applies to the Klein-Gordon field coupled to an external electromagnetic field.

- Even restricting to a free scalar field on a nontrivial geometry, the action that we constructed is not the most general one that is quadratic in ϕ. For example, we could have included in the action the term

$$S' = \int d^4x \sqrt{g} \left(-\frac{1}{2} \xi R(x) \phi^2(x) \right),$$

where R is the scalar curvature. Then the field equation would become

$$\left[\nabla^\mu \nabla_\mu + m^2 + \xi R(x) \right] \phi(x) = 0$$

More complicated terms in the field equation involving other invariants constructed from the curvature could also be included (but would be expected to be suppressed by powers of $G \sim M_{\text{Planck}}^{-2}$ and would be negligible for curvature small in Planck units). For any such field equation, we can construct a Klein-Gordon inner product. But for now, we will ignore any such additional dependence on the background geometry and continue to consider the equation

$$\left(\nabla^\mu \nabla_\mu + m^2\right) \varphi = 0,$$

which already serves to illustrate some of the features of QFT on a nontrivial background.

- In constructing a quantum theory, we will initially ignore the "backreaction" of the field ϕ on the geomemtry, expressed by $G^{\mu\nu} = -8\pi G T^{\mu\nu}$. We will consider the geometry to be a classical source that is not influenced by the (quantum) field ϕ. Later, we will attempt to discuss some backreaction effects.

Canonical Quantization

On a globally hyperbolic spacetime, which has a well-behaved globally defined time coordinate, we can perform canonical quantization of the classical free Klein-Gordon theory. We choose time slices and then impose

$$[\phi(x), \dot{\phi}(y)]_{\text{e.t.}} = i\delta^3(\vec{x} - \vec{y})$$
$$[\phi(x), \phi(y)]_{\text{e.t.}} = 0 = [\dot{\phi}(x), \dot{\phi}(y)]$$

We may put this in a more covariant-looking form by denoting a Cauchy surface by Σ, and letting n^μ be the normalized forward-pointing normal to $Sigma$. Then

$$[\phi(x), n^\mu \partial_\mu \phi(y)]_\Sigma = i\frac{1}{\sqrt{h}}\delta^3(\vec{x} - \vec{y})$$
$$[\phi(x), \phi(y)]_\Sigma = 0$$
$$[n^\mu \partial_\mu \phi(x), n^\nu \partial_\nu \phi(y)]_\Sigma = 0$$

(Henceforth, all commutators are evaluated for two fields on the slice Σ, and $\frac{1}{\sqrt{h}}\delta^3(\vec{x} - \vec{y})$ is the appropriate δ function normalization for integration against the invariant induced volume element $\mathrm{d}^3\, x\sqrt{h}$.)

In fact, if we impose the canonical commutation relations (CCR) on any spacelike Σ, then they are automatically satisfied on every other spacelike surface, provided that $\phi(x)$ satisfies the KG equation. To see this, we first show:

- ϕ satisfies CCR on Σ if and only if $[(f, \phi)_\Sigma, (g, \phi)_\Sigma] = -\left(f, g^*\right)_\Sigma$ for any two solutions f and g to the KG equation.

Thus, if ϕ satisfies the KG equation, we can use the slice independence of the inner product on Σ and show that:
ϕ satisfies CCR on $\Sigma \Longleftrightarrow \phi$ satisfies CCR on Σ', where Σ and Σ' are any two spacelike slices.

To show the only if part of the first statement above, recall

$$(f,g)_\Sigma \equiv i\int_\Sigma \mathrm{d}^3\, x\sqrt{h}n^\mu \left(f^*\partial_\mu g - \partial_\mu f^* g\right)$$

and evaluate

$$\begin{aligned}
&[(f,\phi)_\Sigma, (g,\phi)_\Sigma] \\
&= \left[i\int_\Sigma d^3x\sqrt{h}n^\mu \left(f^*\partial_\mu\phi - \partial_\mu f^*\phi\right), i\int d^3x'\sqrt{h'}n^\nu \left(g^*\partial_\nu\phi - \partial_\nu g^*\phi\right)\right] \\
&= -\int_\Sigma d^3x\sqrt{h}\int_\Sigma d^3x'\sqrt{h'}\,\big[f^*(x)(-n^\nu\partial_\nu g^*(x'))\,[n^\mu\partial_\mu(\phi(x),\phi(y)] - n^\mu_\mu\partial_\mu f^*(x)g^*\left(x'\right)[\phi(x), n^\nu\partial_\nu\phi(y)]\big] \\
&= i\int_\Sigma d^3x\sqrt{h}n^\mu \left(\partial_\mu f(x)^* g^*(x) - f^*(x)\partial_\mu g^*(x)\right)\Big] \\
&= -(f,g^*)_\Sigma
\end{aligned}$$

(To see the if part, we note that we can chooose f, g and their normal derivatives to be arbitrary functions on Σ. From this initial data we obtain solutions to KG equation that are globally defined in spacetime, if the spacetime is globally hyperbolic.)

Thus for a field that satisfies the KG equation, we find that:

(i) If the CCR are imposed on any spacelike slice, they hold on all slices. The quantum field theory tdoes not depend on how we slice the spacetime.

(ii) The theory is causal in the sense

$$[\phi(x), \phi(y)] = 0$$

whenever there is a spacelike slice that contains both x and y. (For globally hyperbolic spacetimes, this slice presumably exists as there are no timelike or null curves connecting x and y.)

Now we wish to proceed with the construction of the Fock space, the Hilbert space of this theory. As was emphasized in the discussion of the flat spacetime case, the construction of the Fock space does not require that the notion of a particle apply. We need only to be able to divide the space of solutions of the KG equation into subspaces with positive definite and negative definite KG norm.

The existence of a *complete* basis for the solutions to the KG equation whose inner product on Σ satisfies

$$\begin{aligned}
(u_i, u_j)_\Sigma &= \delta_{ij} \\
\left(u_i, u_j^*\right)_\Sigma &= 0 \\
\left(u_i^*, u_j^*\right)_\Sigma &= -\delta_{ij}
\end{aligned}$$

follows from the property that initial data on Σ determines a unique solution, for arbitrary initial data can be expanded in such a basis. (Note that we are now using a schematic notation in which discrete normalization of the solutions is assumed.) This is particularly easy to see in the case where the slice Σ has the topology of $\mathbb{R}^3$. In that case, we can smoothly deform the geometry so that it is flat in the sufficiently distant past on Σ.

Then we can choose such a basis in the flat region and propagate it ahead to Σ to get the desired basis in the vicinity of Σ. (The KG inner product is basis independent and depends only on the solution and its first derivative on the slice.)

Now, if we expand the field ϕ in terms of this basis

$$\phi = \sum_i \left(u_i a_i + u_i^* a_i^\dagger\right)$$

we have

$$(u_i, \phi) = a_i$$
$$-\left(u_i{}^*, \phi\right) = a_i{}^\dagger$$

evaluated on any slice. Therefore, the CCR in the form

$$[(f, \phi), (g, \phi)] = -\left(f, g^*\right)$$

implies

$$\begin{aligned}
(a_i, a_j) &= -\left(u_i, u_j^*\right) = 0 \\
\left(a_i^\dagger, a_j^\dagger\right) &= 0 \\
\left(a_i, a_j^\dagger\right) &= -\left(u_i, -u_j\right) = \delta_{ij}
\end{aligned}$$

That is, the $a_i, a_i^\dagger$ are conventionally normalized creation and annihilation operators. And since $[(f, \phi), (g, \phi)] = -\left(f, g^*\right)$ for a complete basis of solutions implies the CCR on any spacelike Σ, we could just as well assume the $aa^\dagger$ commutators and then infer the canonical commutators.

That is, an alternative to canonical quantization is to choose a complete basis $\{u, u^*\}$ of solutions of the KG equation, and construct $\mathcal{H}^{(1)}$, the Hilbert space spanned by the u_i. Then extend to the Fock space $\mathcal{H}$ and define a_i on $\mathcal{H}$. Finally, we can construct the field ϕ on $\mathcal{H}$, which we have shown is local, i.e satisfies $[\phi(x), \phi(y)] = 0$ if x, y lies in a spacelike slice.

In the construction of the Fock space basis, there is, however, an ambiguity. There are many ways to choose the basis $\{u_i\}$ of solutions with positive Klein-Gordon norm. For example, if u satisfies

$$(u, u) = 1, \quad (u, u^*) = 0, \quad (u^*, u^*) = -1$$

then

$$u' = \cosh\theta u + \sinh\theta u^*$$
$$u'^* = \sinh\theta u + \cosh\theta u^*$$

satisfies

$$\left(u', u'\right) = \cosh^2\theta - \sinh^2\theta = 1$$
$$\left(u', u'\right)(x) = \cosh\theta\sinh\theta - \sinh\theta\cosh\theta = 0$$

A linear combination of positive and negative norm solutions is just as acceptable as a basis as u_i.

There is a *natural* way to decompose the space of solutions to the KG equation into subspaces on which the KG inner product is positive definite and negative definite, respectively, only in the special case of a stationary spacetime (like flat space). We say that the spacetime is stationary if the time coordinate t can be chosen so that the metric is $t-$independent. Then $\frac{\partial}{\partial t}$ generates a *symmetry* of the geometry and is said to be a timelike "Killing vector" (the spacetime is invariant under time translations).

Since time translation is a symmetry of the equation, if $u(t,x)$ is a solution to the KG equation, then so is

$$u(t+dt,\vec{x}) = u(t,\vec{x}) + dt\frac{\partial}{\partial t}u(t,\vec{x}).$$

Therefore, the solutions transform as a representation of the time translation group, and we may decompose this representation into one-dimensional *irreducible* subrepresentations. In other words, the operator

$$H = i\frac{\partial}{\partial t}$$

preserves the space of solutions, and we can diagonalize H on this space:

$$Hu_k = \omega_k u_k$$
$$Hu_k^* = -\omega_k u_k^*$$

where ω_k is the frequency of the solution. The solutions then have the form $u_k(t,x) = e^{-i\omega_k t}v(\vec{x})$.

From $(f,g) = i\int d^3x\sqrt{h(t)}\left(f^*(t)\dot{g}(t) - \dot{f}^*(t)g(t)\right)$, we see that, since the inner product is independent of t, we have for $\dot{h}(t) = 0$,

$$(f(t),g(t))_t = (f(t+dt),g(t+dt))_t$$
$$= (f,g)_t + dt[(\dot{f},g) + (f,\dot{g})]$$
$$\Rightarrow (\dot{f},g) + (f,\dot{g}) = 0$$

So for solutions of definite frequency $\dot{u}_k = -i\omega_k u_k$ we have

$$i(\omega_k - \omega_j)(u_k,u_j) = 0$$

This shows that solutions of distinct frequency are *orthogonal* in the KG inner product.

Since the inner product

$$(u_k, u_j)_{t=0} = (\omega_k + \omega_j) \int_{t=0} d^3x \, v_k(\vec{x})^* v_j(\vec{x})$$

is evidently positive definite for positive frequency solutions, we have found a basis (the positive frequency basis) such that

$$\begin{aligned}(u_i, u_j) &= \delta_{ij} \\ (u_i, u_j^*) &= 0 \\ (u_i^*, u_j^*) &= -\delta_{ij}\end{aligned}$$

Acting on this basis, the operator H is nonnegative. If we define operators a_i and a state $|0\rangle$ such that

$$a_i|0\rangle = 0, \quad |i\rangle = a_i^\dagger|0\rangle \text{ where } \langle i|j\rangle = \delta_{ij}$$

We have

$$\left[a_i, a_j^+\right] = \delta_{ij}, \quad \left[a_i, a_j'\right] = 0, \quad [a^+, a^+] = 0$$

acting on Fock space

$$H^{(0)} \oplus H^{(1)} \oplus H^{(2)} \oplus \cdots$$

and the Hamiltonian H has the diagonalization

$$H = \sum_k \omega_k a_k^+ a_k$$

But in general, in the case of a nonstationary spacetime, there is no natural choice for the positive norm subspace of the space of KG solutions, and hence no natural Fock space vacuum. The "correct" choice would be motivated not by mathematics but by the *physical* question we are trying to ask in a particular context.

In the case of a black hole, the geometry is stationary, but it is stationary only outside the event horizon. (Inside the horizon, the light cones tip inward, and the Killing vector becomes spacelike.) In this case, the issue of a vacuum for the stationary region outside the horizon amounts to imposing appropriate boundary conditions on the fields at the horizon.

A situation in which the spacetime is not stationary, but there are (two) natural choices for a Fock space vacuum is the case on a spacetime that becomes asymptotically stationary in the past or future (or both).

If $\{u_i, u_i^*\}$ is a standard basis for the solutions to the KG equation on flat space, then we may choose solutions to the exact KG equation such that

$$p_i \to u_i \text{ in the } \textit{past.}$$

Then $(p_i, p_j) = \delta_{ij}, (p_i, p_j^*) = 0 \quad (p_i^*, p_j^*) = -\delta_{ij}$ on any slice, since this is true for a slice in the asymptotic past, and the inner product is independent of the slice. Similarly we may choose a basis

$$f_i \to u_i \text{ in the } \textit{future}$$

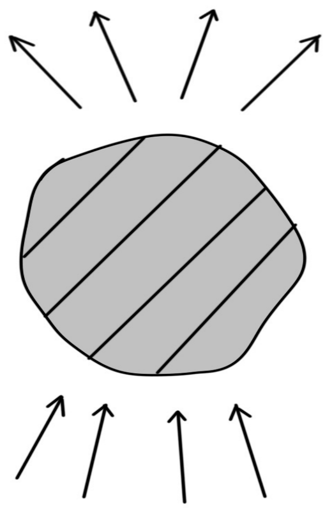

Figure 4. A situation where the spacetime is stationary in the past and future.

that becomes positive frequency in the future. These two bases need not coincide. A basis of positive frequency solutions in the past will propagate to a *positive norm* basis in the future, but not necessarily to a basis of *positive frequency* solutions in the future. Hence, the incoming Fock space vacuum may evolve to a state that is not a vacuum in the future– the fluctuating geometry can create particles.

In this situation, where the spacetime is asymptotically stationary (in particular, flat) in the past and future, an S matrix can be defined that relates the past and future Fock space basis - and hence gives the amplitude for an incoming particle state to "scatter" off the geometry, yielding an outgoing particle state.

Let $|\psi\rangle$ denote a Fock space state for QFT on flat spacetime. Then we denote by $|\psi_{\text{in}}\rangle, |t_{\text{out}}\rangle$ the states of the theory on a nontrivial background that asymptotically approach $|\psi\rangle$ in the past, future respectively. Then we define S by

$$S|\psi_{\text{out}}\rangle = |\psi_{\text{in}}\rangle$$

S will then be a unitary operator (it preserves the inner product - what comes out – goes out). Thus $|\psi_{\text{out}}\rangle = S^{-1}|\psi_{\text{in}}\rangle \Rightarrow \langle\psi_{\text{out}}| = \langle\psi_{\text{in}}|\left(S^{-1}\right)^{\dagger} = \langle\psi_{\text{in}}|S$.
Then we have

$$\begin{aligned}\langle\chi_{\text{out}}|\psi_{\text{out}}\rangle &= \langle\chi_{\text{out}}|S|\psi_{\text{out}}\rangle \\ &= \langle\chi_{\text{in}}|S|\psi_{\text{in}}\rangle\end{aligned}$$

This is an inner product between states of the theory on a trivial background, if evolved in the asymptotic past or future.

Remarks

We have defined S as a change of the Fock basis in the Hilbert space of the theory.
$|\psi_{\text{out}}\rangle \in \mathcal{H}$ resembles $|\psi\rangle \in \mathcal{H}^{\text{out}}$ in future
$|\psi_{\text{in}}\rangle \in \mathcal{H}$ resembles $|\psi\rangle \in \mathcal{H}^{\text{in}}$ in past.

Then $S|\psi_{\text{out}}\rangle = |\psi_{\text{in}}\rangle$.

An alternative approach is to define $\hat{S} : \mathcal{H}^{\text{in}} \to \mathcal{H}^{\text{out}}$ so that:

$$|\psi_{\text{in}}\rangle = |\chi_{\text{out}}\rangle \Rightarrow \hat{S}|\psi\rangle = |\chi\rangle$$

Then

$$|i_{\text{in}}\rangle = S|i_{\text{out}}\rangle = \sum_j |j_{\text{out}}\rangle\langle j_{\text{out}}|S|i_{\text{out}}\rangle$$

$$\Rightarrow \hat{S}|i\rangle = \sum_j |j\rangle\langle j_{\text{out}}|S|i_{\text{out}}\rangle$$

and thus,

$$\begin{aligned}\langle j|\hat{S}|i\rangle &= \langle j_{\text{in}}|S|i_{\text{out}}\rangle \\ &= \langle j_{\text{in}}|S|i_{\text{in}}\rangle\end{aligned}$$

In the language we have used here, we have:

$$\phi = \sum_i \left(p_i a_i^{\text{in}} + p_i^* a_i^{\text{in}\dagger}\right) = \sum_i \left(f_i a_i^{\text{out}} + f_i^* a_i^{\text{out}\dagger}\right)$$

where $\phi : \mathcal{H} \to \mathcal{H}$.

In the alternate language, $a^{\text{in:}}$ $\mathcal{H}^{\text{in}} \to \mathcal{H}^{\text{in}}$ and $a^{\text{out:}}$ $\mathcal{H}^{\text{out}} \to \mathcal{H}^{\text{out}}$.

These are related by

$$S\left[\sum_i \left(p_i a_i^{\text{in}} + p_i^* a_i^{\text{in}\dagger}\right)\right] S^{-1} = \sum_i \left(f_i a_i^{\text{out}} + f_i^* a_i^{\text{out}\dagger}\right)$$

and so

$$S\begin{pmatrix}a^{\mathrm{in}} & a^{\mathrm{in}\dagger}\end{pmatrix}S^{-1} = \begin{pmatrix}a^{\mathrm{out}} & a^{\mathrm{out}\dagger}\end{pmatrix}\begin{pmatrix}\alpha & \beta \\ \beta^* & \alpha^*\end{pmatrix}$$

$$\Rightarrow S\begin{pmatrix}a^{\mathrm{in}} \\ a^{\mathrm{in}\dagger}\end{pmatrix}S^{-1} = \begin{pmatrix}\alpha^\dagger & \beta^\dagger \\ \beta^\dagger & \alpha^\dagger\end{pmatrix}\begin{pmatrix}a^{\mathrm{out}} \\ a^{\mathrm{out}\dagger}\end{pmatrix}$$

$$\text{or } S^{-1}\begin{pmatrix}a^{\mathrm{out}} \\ a^{\mathrm{out}\dagger}\end{pmatrix}S = \begin{pmatrix}\alpha^* & -\beta^* \\ -\beta & \alpha\end{pmatrix}\begin{pmatrix}a^{\mathrm{in}} \\ a^{\mathrm{in}\dagger}\end{pmatrix}$$

This is precisely the same equation that we have for S later on, provided we identify a^{in} and a^{out}. In making this identification, we are recognizing the natural isomorphism $\mathcal{H}^{\mathrm{in}} \to \mathcal{H}^{\mathrm{out}}$ and that we must make use of this isomorphism to define S matrix elements (since $\mathcal{H}^{\mathrm{in}}$ and $\mathcal{H}^{\mathrm{out}}$ are otherwise regarded as distinct spaces).

Let $|i\rangle$ denote a complete basis for the Fock space of theory on trivial background (not just for $\mathcal{H}^{(1)}$, but all of Fock space). Then, the S-matrix has the representation:

$$S = \sum_i |i, \mathrm{in}\rangle\langle i, \mathrm{out}|$$

(This ensures $S|i, \mathrm{out}\rangle = |i, \mathrm{in}\rangle$ acting on basis). Therefore,

$$S^{-1} = S^\dagger = \sum_i |i, \mathrm{out}\rangle\langle i, \mathrm{in}|$$

If θ^{in} is any operator, then

$$\langle i, \mathrm{in}|\theta^{\mathrm{in}}|j, \mathrm{in}\rangle = \langle i, \mathrm{out}|S^{-1}\theta^{\mathrm{in}}S|j, \mathrm{out}\rangle$$

or

$$\theta^{\mathrm{out}} = S^{-1}\theta^{\mathrm{in}}S$$

That is, $S^{-1}\theta^{\mathrm{in}}S$ has the same matrix elements between out-states as θ^{in} does between in-states.

We can calculate S if we can solve the KG equation on the nontrivial background. The solutions f, p solve the flat space equation in past and future; since $\{u_i, u_i^*\}$ form a complete basis for solutions, we have:

$$f_i \to u_i \text{ in future}$$

$$f_i \to \alpha_{ij}u_j + \beta_{ij}u_j^* \text{ in the past}$$

for appropriate matrices α, β.

Similarly,

$$p_i \to u_i \text{ in the past}$$

$$p_i \to \gamma_{ij} u_j + \delta_{ij} u_j^* \text{ in the future}$$

But because the KG equation is linear and homogeneous even where the background is nontrivial, we have:

$$\begin{aligned} f_i &= \alpha_{ij} p_j + \beta_{ij} p_j^* \\ p_i &= \gamma_{ij} f_j + \delta_{ij} f_j^* \end{aligned}$$

By expanding ϕ in terms of both bases, we find:

$$\begin{aligned} \phi &= \sum_i \left(p_i a_i^{\text{in}} + p_i^* a_i^{\text{in}\dagger} \right) \\ &= \sum_j \left(f_i a_i^{\text{out}} + f_i^* a_i^{\text{out}\dagger} \right) \end{aligned}$$

and thus infer a linear relation among $a^{\text{in}}, a^{\text{in}\dagger}$ and $a^{\text{out}}, a^{\text{out}\dagger}$. We may then solve for S by demanding:

$$\begin{aligned} S^{-1} a^{\text{in}} S &= a^{\text{out}} \\ S^{-1} a^{\text{in}\dagger} S &= a^{\text{out}\dagger} \end{aligned}$$

To see how this goes, let's consider the somewhat more general problem of the relation between two Fock space bases obtained by expanding the field in terms of two different orthonormal bases for the KG solutions (that are linearly related).

$$\begin{aligned} u_i' &= \alpha_{ij} u_j + \beta_{ij} u_j^* \\ u_i'^* &= \beta_{ij}^* u_j + \alpha_{ij}^* u_j^* \end{aligned}$$

In matrix notation:

$$\begin{pmatrix} u' \\ u'^* \end{pmatrix} = \begin{pmatrix} \alpha & \beta^* \\ \beta^* & \alpha^* \end{pmatrix} \begin{pmatrix} u \\ u^* \end{pmatrix}$$

If both bases are normalized so that

$$(u_i, u_j) = \delta_{ij}, \quad (u_i^*, u_j) = 0, \quad \left(u_i^*, u_j^*\right) = -\delta_{ij}$$

$$\left(u_i', u_j'\right) = \delta_{ij}', \quad \left(u_i'^*, u_j'\right) = 0, \quad \left(u_i'^*, u_j'^*\right) = -\delta_{ij}$$

then we have

$$\begin{aligned} \delta_{ij} = \left(u_i', u_j'\right) &= \alpha_{ik}^* \alpha_{jl} \delta_{kl} - \beta_{ik}^* \beta_{jl} \delta_{ke} \\ &= \left(\alpha \alpha^\dagger - \beta \beta^\dagger \right)_{ji} \end{aligned}$$

Thus,

$$\boxed{\alpha\alpha^\dagger - \beta\beta^\dagger = \mathbb{1}}$$

Also,

$$0 = (u_i'^*, u_j) = \beta_{ik}\alpha_{jl}\delta_{kl} - \alpha_{ik}\beta_{jl}\delta_{kl}$$
$$\Rightarrow \boxed{\alpha\beta^T - \beta\alpha^T = 0}$$

From these identities, it follows that the left inverse is

$$\begin{pmatrix} \alpha & \beta \\ \alpha^* & \beta^* \end{pmatrix}^{-1} = \begin{pmatrix} \alpha^\dagger & -\beta^\dagger \\ -\beta^\dagger & \alpha^\dagger \end{pmatrix}$$

(The inverse is unique if it exists. Also this is the right inverse as well as left inverse as we will see from additional identities shortly).

And therefore,

$$\begin{pmatrix} u \\ u^* \end{pmatrix} = \begin{pmatrix} \alpha^\dagger & -\beta^T \\ -\beta^\dagger & \alpha^T \end{pmatrix} \begin{pmatrix} u' \\ u'^* \end{pmatrix}$$

Compare now the two mode expansions:

$$\phi = \sum_i \left(u_i a_i + u_i^* a_i^\dagger \right) = \left(a \ a^\dagger \right) \begin{pmatrix} u \\ u^* \end{pmatrix}$$
$$= \sum_i \left(u_i' a_i' + u_i'^* a_i^\dagger \right) = \left(a' \ a'^\dagger \right) \begin{pmatrix} u' \\ u'^* \end{pmatrix}$$

Substituting for u', u'^* in terms of u, u^* and vice versa gives

$$\left(a \ a^\dagger \right) \begin{pmatrix} u \\ u^* \end{pmatrix} = \left(a' \ a'^\dagger \right) \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \begin{pmatrix} u \\ u^* \end{pmatrix}$$
$$\left(a'^+ a'^\dagger \right) \begin{pmatrix} u' \\ u'^* \end{pmatrix} = \left(a \ a^\dagger \right) \begin{pmatrix} \alpha^\dagger & -\beta^\dagger \\ -\beta^\dagger & \alpha^\dagger \end{pmatrix} \begin{pmatrix} u' \\ u'^* \end{pmatrix}$$

Therefore, since the bases are complete and orthonormal (e.g., we can isolate coefficients by taking KG inner product), we have we have

$$\begin{pmatrix} a & a^\dagger \end{pmatrix} = \begin{pmatrix} a' & a'^\dagger \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$$

$$\begin{pmatrix} a'^\dagger a'^\dagger \end{pmatrix} = \begin{pmatrix} a & a^\dagger \end{pmatrix} \begin{pmatrix} \alpha^\dagger & -\beta^\dagger \\ -\beta^\dagger & \alpha^\dagger \end{pmatrix}$$

and taking transposes

$$\boxed{\begin{pmatrix} a' \\ a'^\dagger \end{pmatrix} = \begin{pmatrix} \alpha^* & -\beta^* \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} \alpha^\dagger & \beta^\dagger \\ \beta^\dagger & \alpha^\dagger \end{pmatrix} \begin{pmatrix} a' \\ a'^\dagger \end{pmatrix}}$$

Since $\begin{pmatrix} \alpha^\dagger & \beta^\dagger \\ \beta^\dagger & \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \alpha^* & -\beta^* \\ -\beta & \alpha \end{pmatrix}^{-1}$,
we have the additional identities:

$$\alpha^T \alpha^* - \beta^\dagger \beta = \mathbb{1}$$
$$\alpha^T \beta^* - \beta^\dagger \alpha = 0$$

Since the u, u^*'s and u', u'^*'s are normalized, both the $a, a^\dagger$ and $a', a'^\dagger$ satisfy the standard commutation relations. The transformation $(a, a^\dagger) \to (a', a'^\dagger)$ is a *canonical transformation*—a change of variables that preserves the commutation relations. A canonical transformation that uses linear combinations of $a, a^\dagger$ is called a Bogoliubov transformation.

For $\beta \neq 0$, we have changed the positive norm subspace of the space of solutions to KG equation. Nonetheless, the two Hilbert spaces are related by a unitary transformation, because a canonical transformation can be implemented by a unitary transformation acting on the Hilbert space.(Actually, for a system with an infinite number of degrees of freedom, this is true only subject to certain conditions that will emerge from the calculation below.)

As described earlier, we may define a unitary change of basis by:

$$U|\psi'\rangle = |\psi\rangle$$

In which case:

$$U^{-1} a U = a'$$
$$U^{-1} a^\dagger U = a'^\dagger$$

(Note: U will be unitary if it preserves the norm of $|0\rangle$–then, since it preserves commutators, its preserves norms of all Fock states. From these equations and the Bogoliubov transformation, we can solve for U in terms of a, a'. It takes the same form in both representations, since $\langle\psi'|U|\psi'\rangle = \langle\psi|U|\psi\rangle$.)

It is convenient to express U as a normal ordered function of $a, a^\dagger$:

$$U =: U(a, a^\dagger) :$$

(where the double dots denote normal ordering). Normal-ordered means that all a operators lie to the right of all $a^\dagger$ operators. To solve:

$$\begin{aligned} aU &= Ua' = U(\alpha^* a - \beta^* a^\dagger) \\ a^\dagger U &= Ua'^\dagger = U(-\beta a + \alpha a^\dagger) \end{aligned}$$

We note that operators $a, a^\dagger$ act on normal-ordered functions as:

$$\begin{aligned} a_i : \theta : &=: (a_i + \frac{\partial}{\partial a_i}\dagger)\theta : \\ a_i^\dagger : \theta : &=: a_i^\dagger \theta : \\ : \theta : a_i : &= \ a_i \theta : \\ : \theta : a_i^\dagger : &=: (a_i^\dagger + \frac{\partial}{\partial a_i})\theta : \end{aligned}$$

since

$$\begin{aligned} [a_i, f(a^\dagger)] &= \frac{\partial}{\partial \alpha_i^\dagger} f(a^\dagger) \\ [f(a), a_i^\dagger] &= \frac{\partial}{\partial a_i} f(a) \end{aligned}$$

So we must find a function $U(a, a^\dagger)$ satisfying:

1. $\left(a + \frac{\partial}{\partial a^\dagger}\right) U = \left[\alpha^* a - \beta^* \left(a^\dagger + \frac{\partial}{\partial a}\right)\right] U$
2. $a^\dagger U = \left[-\beta a + \alpha \left(a^\dagger + \frac{\partial}{\partial a}\right)\right] U$

(Normal ordering is now understood and not explicitly indicated.)

We solve this by means of the ansatz:

$$\begin{aligned} U &= C \exp\left[\frac{1}{2}\left(a\, a^\dagger\right) \begin{matrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{matrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}\right] \\ &= C \exp\left[\frac{1}{2}\left(aM_{11}a + aM_{12}a^\dagger + a^\dagger M_{21} a + a^\dagger M_{22} a^\dagger\right)\right] \end{aligned}$$

where we may assume without loss of generality:

$$M_{11} = M_{11}^T, \quad M_{22} = M_{22}^T, \quad M_{12} = M_{21}^T$$

Then:

$$\frac{\partial}{\partial a}U = \left(M_{11}a + M_{12}a^\dagger\right)U$$
$$\frac{\partial}{\partial a^\dagger}U = \left(M_{21}a + M_{22}a^\dagger\right)U$$

And we have the following algebraic equations:
(i) $\left(a + M_{21}a + M_{22}a^\dagger\right) = \alpha^* a - \beta^*\left(a^\dagger + M_{11}a + M_{12}a^\dagger\right)$
(ii) $a^\dagger = -\beta a + \alpha\left(a^\dagger + M_{11}a + M_{12}a^\dagger\right)$
Since the coefficients of a and $a^\dagger$ must vanish, (ii) implies:

$$\begin{array}{l} \mathbb{1} = \alpha + \alpha M_{12} \\ 0 = -\beta + \alpha M_{11} \end{array} \Rightarrow \boxed{\begin{array}{l} M_{12} = \alpha^{-1} - \mathbb{1} \\ M_{11} = \alpha^{-1}\beta \end{array}}$$

How do we know that α is invertible? This follows from the identity:

$$\alpha\alpha^\dagger = \mathbb{1} + \beta\beta^\dagger$$

which shows that $\alpha\alpha^\dagger$ has no zero eigenvalue. Thus, $\langle\psi|\alpha\alpha^\dagger|\psi\rangle = \|\alpha^\dagger|\psi\rangle\|^2 > 0$. $\alpha^\dagger$ has trivial kernel, and therefore, the range of α is the entire space. Furthermore, $\left(\alpha^\dagger\alpha\right)^* = \mathbb{1} + \beta^\dagger\beta$ shows that the kernel $\alpha = 0$ –so α has a left and right inverse.

From (i), we find:

$$M_{22} = -\beta^* - \beta^* M_{12} = -\beta^*\alpha^{-1}$$
$$\mathbb{1} + M_{21} = \alpha^* - \beta^* M_{11} = \alpha^* - \beta^*\alpha^{-1}\beta$$

or

$$\boxed{M_{22} = -\beta^*\alpha^{-1}, \quad M_{21} = -\mathbb{1} + \alpha^* - \beta^*\alpha^{-1}\beta}$$

Now, we must check that this solution is consistent with the assumptions:

$$M_{11} = M_{11}^T, \quad M_{22} = M_{22}^T, \quad M_{21} = M_{12}^T$$

These relations actually follow from the identities:

$$\begin{array}{cc} \alpha\alpha^\dagger - \beta\beta^\dagger = \mathbb{1} & \alpha^T\alpha^* - \beta^\dagger\beta = \mathbb{1} \\ \beta\alpha^T = \alpha\beta^T & \beta^\dagger\alpha = \alpha^T\beta^* \end{array}$$

E.g., from

$$\beta\alpha^T = \alpha\beta^T \text{ we have } \alpha^{-1}\beta = \beta^T(\alpha^T)^{-1} = \left(\alpha^{-1}\beta\right)^T$$
$$\beta^\dagger\alpha = \alpha^T\beta^* \Rightarrow \beta^*\alpha^{-1} = \left(\alpha^T\right)^{-1}\beta^\dagger = \left(\beta^*\alpha^{-1}\right)^T$$

And from

$$\mathbb{1} = \alpha^T \alpha^* - \beta^\dagger \beta = \alpha^T \alpha^* - \left(\alpha^T \beta^* \alpha^{-1}\right) \beta,$$

We have

$$\left(\alpha^T\right)^{-1} = \alpha^* - \beta^* \alpha^{-1} \beta,$$

so that $M_{12}^T = M_{21}$.

We have now found:

$$\boxed{U = C : \exp\left[\frac{1}{2} a \left(\alpha^{-1}\beta\right) a + a \left(\alpha^{-1} - \mathbb{1}\right) a^\dagger + \frac{1}{2} a^\dagger \left(-\beta^* \alpha^{-1}\right) a^\dagger\right] :}$$

To complete the calculation of U, we must find the constant C. We may determine C up to a phase by requiring that U is unitary, so:

$$\left|0'\right\rangle = U^\dagger |0\rangle \Rightarrow \left\langle 0' | 0' \right\rangle = \langle 0|0\rangle = \mathbb{1}$$

where $|0\rangle$ is the vacuum satisfying $a_i|0\rangle = 0$. Since the adjoint is a normal ordered operator and is normal ordered, we have:

$$U^\dagger = C^* : \exp\left[\frac{1}{2} a^\dagger \left(\alpha^{-1}\beta\right)^* a^\dagger + \cdots\right] :$$

and $U^\dagger|0\rangle = C^* \exp\left[\frac{1}{2} a^\dagger \left(\alpha^{-1}\beta\right)^* a^\dagger\right] |0\rangle$

Now, we invoke the identity:

$$\left\langle 0 \middle| \exp\left(\frac{1}{2} a M a\right) \exp\left(\frac{1}{2} a^\dagger M^* a^\dagger\right) \middle| 0 \right\rangle$$
$$= \left[\det\left(\mathbb{1} - M M^*\right)\right]^{-\frac{1}{2}}, \quad \text{where } M = M^T.$$

(We will return to the derivation of this identity shortly.)

Thus:

$$\mathbb{1} = |C|^2 \left(\det\left[\mathbb{1} - \alpha^{-1}\beta \left(\alpha^{-1}\beta\right)^*\right]\right)^{-\frac{1}{2}}$$

We can simplify the determinant by recalling:

$$\alpha^\dagger \alpha - \beta^T \beta^* = \mathbb{1}, \quad \alpha^\dagger \beta = \beta^T \alpha^*$$

$$\Rightarrow \mathbb{1} = \alpha^\dagger \alpha - \alpha + \beta \left(\alpha^*\right)^{-1} \beta^*$$

$$\Rightarrow \left(\alpha^\dagger \alpha\right)^{-1} = \mathbb{1} - \alpha^{-1}\beta \left(\alpha^{-1}\beta\right)^*$$

So we have $|C|^2 = (\det(\alpha \dagger \alpha))^{-\frac{1}{2}}$, and we have determined C up to a phase:

$$|C| = \left(\det \alpha^\dagger \alpha\right)^{-\frac{1}{4}}$$

We will not attempt to determine the phase of C. This phase is of little relevance. Moreover, it is subect to ambiguities concerning how the renormalized energy-momentum $T^{\mu\nu}$ is defined, as we will discuss later.

In the case of an asymptotically flat spacetime, we have found the S-matrix:

$$\boxed{S = (\text{phase})(\det \alpha^\dagger \alpha)^{-\frac{1}{4}} : \exp\left[\frac{1}{2} a^{\text{in}}(\alpha^{-1}\beta)a^{\text{in}} + a^{\text{in}}(\alpha^{-1} - \mathbb{1})a^{\text{in}\dagger} + \frac{1}{2} a^{\text{in}\dagger}(-\beta^*\alpha^{-1})a^{\text{in}\dagger}\right] :}$$

It lhas the same form when exoressed in terms of a^{out} , $a^{\text{out}\dagger}$, since:

$$\langle \psi_{\text{in}} | S | \chi_{\text{in}} \rangle = \langle \psi_{\text{out}} | S | \chi_{\text{out}} \rangle \rangle$$

We have:

$$|\langle 0_{\text{out}} | 0_{\text{ in}} \rangle|^2 = \left(\det \alpha^\dagger \alpha\right)^{-\frac{1}{2}}$$

Note that, for the construction of a unitary S-matrix to be possible, we must have $(\alpha^\dagger\alpha) < \infty$, so $|0_{\text{ out}}\rangle$ must have a nonzero overlap with $|0_{\text{ in}}\rangle$. We can state this criterion in a somewhat more physical way by noting that:

$$\begin{aligned} N_i &= \langle 0_{\text{in}} | \underbrace{a_i^{\text{out }\dagger} a_i^{\text{ou}}}_{\text{not summed}} |0_{\text{ n}}\rangle \\ &= \langle 0_{\text{in}} | \left(-\beta_{ij} a_j^{\text{in}}\right)\left(-\beta_{ik}^* a_k^{\text{in}}\right) |0_{\text{in}}\rangle \\ &= \left(\beta\beta^\dagger\right)_{ii} = \sum_j |\beta_{ij}|^2 \end{aligned}$$

This is the expectation value of the number of particles of type i produced by the geometry, when the incoming state is the vacuum. The sum over i gives the total particle number, $N = \sum_i N_i = \text{Tr}(\beta\beta^\dagger)$.

And since $\alpha\alpha^\dagger = \mathbb{1} + \beta\beta^\dagger$, the condition that $\det(\alpha\alpha^\dagger) = \det\left(\mathbb{1} + \beta\beta^\dagger\right) < \infty$ is precisely $N < \infty$.

The canonical transformation $\left(a^{\text{in}}, a^{\text{in}\dagger}\right) \to \left(a^{\text{out}}, a^{\text{out}\dagger}\right)$ *cannot* be implemented by a unitary operator if the $|0\rangle_{\text{in}}$ vacuum is a state with an indefinite number of particles when expanded in terms of the out Fock basis.

(This may happen in principle if there are massless particles and many soft particles, and the many-soft particles are produced by the fluctuating geometry. It does not happen if the (smooth) spacetime is flat outside a compact region, for fluctuating quantum geometry may compose soft particles, see R. Wald, Ann. Phys. 118(1979)490, "Existence of the S-matrix in

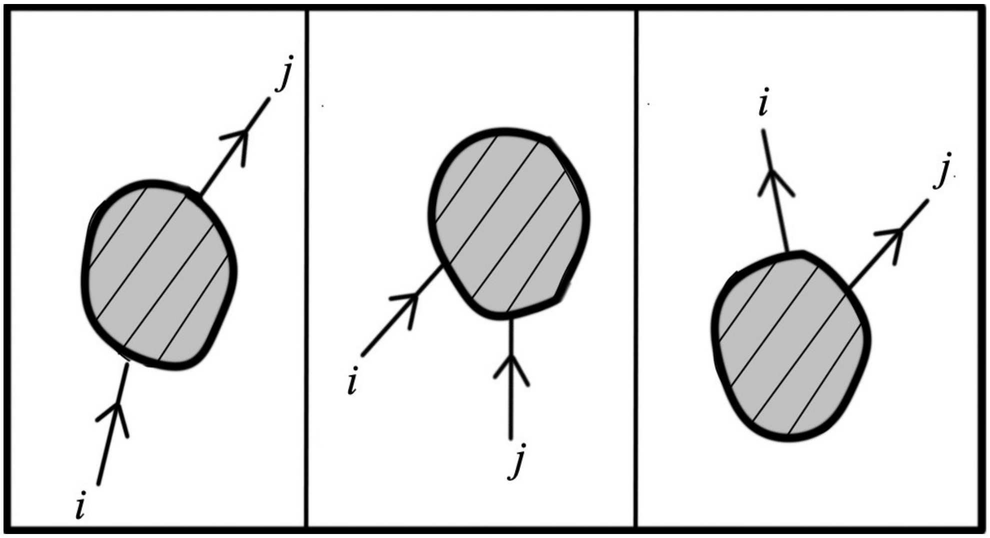

Figure 5. Left: Particle 'scatter' off geometry Center: Particle annihilation by geometry RIght: Particle creation by geometry

QET in Curved Spacetime".)

Some other S-matrix elements are:

$$\langle i_{\text{out}}|j_{\text{in}} = \langle 0_{\text{out}}|)_{\text{in}}\rangle \left(\mathbb{1} + \underbrace{\alpha^{-1} - \mathbb{1}}_{\text{"connected part"}}\right)_{ij} = \alpha^{-1}_{ij}$$

An incoming particle may scatter and emerge with its momentum changed (if $\alpha \neq \mathbb{1}$):

$$\langle ij_{\text{out}}|0_{\text{in}}\rangle = \langle 0_{\text{out}}|0_{\text{in}}\rangle \left(-\beta^* \alpha^{-1}\right)_{ij}$$

$$\langle 0_{\text{out}}|ij_{\text{in}}\rangle = \langle 0_{\text{out}}|0_{\text{in}}\rangle \left(\alpha^{-1}\beta\right)_{ij}$$

Particles are created or annihilated only if $\beta \neq 0$ (Bogoliubov transformation mixes positive and negative frequencies). If $\beta = 0$, then α is unitary, and $\langle 0_{\text{out}}|0_{\text{in}}\rangle$ is a phase.

Particles are not created or annihilated singly, but only in pairs. (These could be particle-antiparticle pairs in the case of a complex scalar field.)

It is also easy to extract from our expression for S the many-particle $\to$ many-particle amplitudes. Consider, for example, $\langle i_1 \ldots i_{2n\ \text{out}}|0_{\text{in}}\rangle$

$$= \langle i_1 \ldots i_{2n}|S|0\rangle = \langle i_1 \ldots i_{2n} \left| \frac{1}{n!}\left(\frac{1}{2} a^\dagger V a^\dagger\right)^n \right| 0\rangle$$

where $V = -\beta^* \alpha^{-1}$.

Allowing the $2n$ $a^\dagger$ operators to annihilate (to the left) the $2n$ particles $i_1 \dots i_{2n}$ generates $(2n!)$ terms, each term giving a product $V.V \dots V$ of n matrix elements in the symmetric matrix V. This product depends only on how the $2n$ indices are paired, and each pairing occurs $n!2^n$ times.

This is the number of the $(2n)!$ permutations of indices that leave the pairing unchanged. Thus, the $\frac{1}{n!2^n}$ gets cancelled, and we have:

$$\langle i_1 \dots i_{2n} \text{ out } |0\rangle_{\text{in}}\rangle = V_{i_1,i_2} V_{i_3,i_4} \dots V_{i_{2n-1,1} i_n} + \text{ all other pairings,}$$

there being $(2n)!/(n!2^n)$ terms in the sum.
E.g

$$\langle i_1 \dots i_4 \text{ out } |0\rangle_{\text{in}}\rangle = V_{i_1,i_2} V_{i_3,i_4} + V_{i_1,i_3} V_{i_2,i_4} + V_{i_1,i_4} V_{i_2,i_3}$$

Proof of the Identity

We return now to the derivation of the identity:

$$\left\langle 0 \left| \exp\left(\frac{1}{2} aMa\right) \exp\left(\frac{1}{2} a^] daM^* a^\dagger\right) \right| 0 \right\rangle = \left[\det\left(\mathbb{1} - MM^*\right)\right]^{-\frac{1}{2}} \text{ (where } M = M^T\text{).}$$

The slick way to evaluate such matrix elements is to convert them to Gaussian integrals.

An arbitrary Fock space state can be represented as a function of $a^\dagger$ acting on $|0\rangle$:

$$|\psi\rangle = \psi(a^\dagger)|0\rangle = \sum_{n=0}^{\infty} \sum_{i_1 \dots i_n} \psi^{(n)}_{i_1 \dots i_n} a^\dagger_{i_1} \dots a^\dagger_{i_n} |0\rangle$$

Here $\psi^{(n)}_{i_1 \dots i_n}$ is symmetric under the exchange of indices.

Claim:

$$\langle \chi | \psi \rangle = \frac{\int dada^\dagger \chi^*(a) \psi\left(a^\dagger\right) e^{-a^\dagger a}}{\int dada^\dagger e^{-a^\dagger a}}$$

Here, on the RHS, $a_i, a_i^\dagger$ are complex c-numbers, and:

$$\int dada^\dagger = \int \Pi_i da_i da_i^\dagger$$

is an integral $\int_{-\infty}^{\infty}$ over real and imaginary parts of each a_i.

To verify the claim, it is enough to show (since we can expand in powers of $a^\dagger$):

$$\left\langle 0 \left| a_{i_1} \ldots a_{i_n} a^\dagger_{j_1} \ldots a^\dagger_{j_m} \right| 0 \right\rangle = \frac{\int da da^\dagger a_{i_1} \ldots a_{i_n} a^\dagger_{j_1} \ldots a^\dagger_{j_m} e^{-a^\dagger a}}{\int da da^\dagger e^{-a^\dagger a}}$$

We can derive this identity by evaluating both sides. Commuting a's through $a^\dagger$'s, we find:

$$\left\langle 0 \middle| a_{i_1} \ldots a_{i_n} a^\dagger_{j_1} \ldots a^\dagger_{j_m} \middle| 0 \right\rangle = \begin{cases} 0 & \text{if } (m \neq n) \\ \delta_{i_1, j_1} \ldots \delta_{i_n j_n} + \text{permutatioons (n! terms altogether)} & \text{if } (m = n) \end{cases}$$

To evaluate the integral on the LHS, construct the generating function

$$Z[J] = \int da da^\dagger e^{\overline{J} a} e^{a^\dagger J} e^{-a^\dagger a}.$$

We complete the square:

$$Z[J] = \int da da^\dagger \exp\left[- \left(a^\dagger - \overline{J} \right) (a - J) + \overline{J} J \right]$$

Shift the integral:

$$= e^{\overline{J} J} Z[0]$$

Now

$$\begin{aligned} &\frac{\int da da^\dagger a_{i_1} \ldots a_{i_n} a^\dagger_{j_1} \ldots a^\dagger_{j_m} e^{-a^\dagger a}}{\int da da^\dagger e^{-a^\dagger a}} \\ =&\frac{1}{Z[0]} \frac{\partial}{\partial \overline{J}_{i_1}} \ldots \frac{\partial}{\partial \overline{J}_{i_n}} \frac{\partial}{\partial J_{j_1}} \ldots \frac{\partial}{\partial J_{j_m}} Z[J] \bigg|_{J = \overline{J} = 0} \\ =&\frac{\partial}{\partial \overline{J}_{i_1}} \ldots \frac{\partial}{\partial \overline{J}_{j_m}} e^{\overline{J} J} \bigg|_{J = \overline{J} = 0} \end{aligned}$$

This evidently vanishes for $n \neq m$. For $n = m$, we have:

$$\begin{aligned} &= \frac{\partial}{\partial J_{j_1}} - \frac{\partial}{\partial J_{j_n}} \left(J_{i_1} - J_{i_n} \right) \\ &= \delta_{i_1 j_1} - \delta_{i_n j_n} + \text{permutations} \end{aligned}$$

By means of Wick's trick, we have:

$$\langle 0 \left| \exp\left(\frac{1}{2} a M a \right) \exp\left(\frac{1}{2} a^\dagger M^* a^\dagger \right) \right| 0 \rangle = \frac{\int da da^\dagger \exp\left[\frac{1}{2} \left(a \, a^\dagger \right) \begin{pmatrix} M & \mathbb{1} \\ \mathbb{1} & M^* \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right]}{\int da da^\dagger \exp\left(a^\dagger a \right)}$$

You can evaluate such an integral by changing variables to real $X = \frac{1}{\sqrt{2}}(a + a^\dagger)$ and $Y = \frac{1}{i\sqrt{2}}(a - a^\dagger)$.

A real Gaussian integral.

$$\int dX e^{-\frac{1}{2}XAX} \quad (A = A^T)$$

can be evaluated if A has an orthonormal basis of eigenvectors:

$$Ae_n = \lambda_n e_n$$

By expanding $X = \sum_n X_n e_n$ in this basis, we find:

$$\begin{aligned}\frac{\int dX e^{-\frac{1}{2}X\cdot AX}}{\int dX e^{-\frac{1}{2}X\cdot X}} &= \Pi_n \left[\frac{\int dX_n e^{-\frac{1}{2}X_n\lambda_n X_n}}{\int dX_n e^{-\frac{1}{2}X_n^2}}\right] \\ &= \Pi_n \lambda_n^{-\frac{1}{2}} = (\det A)^{-\frac{1}{2}}\end{aligned}$$

(The integrals converge for $\mathrm{Re}\lambda_n > 0$, and may be defined by analytic continuation otherwise.)

Writing the integral in terms of reall variables and using elementary properties of determinants, we find (exercise):

$$\left\langle 0 \left| \exp\left(\frac{1}{2}aMa\right) \exp\left(\frac{1}{2}a^\dagger M^* a^\dagger\right) \right| 0 \right\rangle = \left[\det \begin{pmatrix} -\mathbb{1} & M^* \\ M & -\mathbb{1} \end{pmatrix}\right]^{-\frac{1}{2}}$$

and:

$$\begin{aligned}\det \begin{pmatrix} \mathbb{1} & M^* \\ M & \mathbb{1} \end{pmatrix} &= \det \begin{pmatrix} \mathbb{1} & 0 \\ -M & \mathbb{1} \end{pmatrix} \det \begin{pmatrix} \mathbb{1} & M^* \\ M & \mathbb{1} \end{pmatrix} \\ &= \det \begin{pmatrix} \mathbb{1} & M^* \\ 0 & \mathbb{1} - MM^* \end{pmatrix} = \det(\mathbb{1} - MM^*)\end{aligned}$$

Which was to be shown.