2. Field theory on Curved Spacetime

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 generally covariant physics. Locally (at sufficiently short distance) spacetime is approximately flat. Our field theory on curved spacetime should reduce to our flat-spacetime theory locally. Because we must consider local physics, it is essential that we describe the 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 the 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 Poincare group. But a curved background will not be Poincare invariant, nor will the quantum theory built on it admit a unitary rep. of the Poincare group. The notion of a particle is an approximate one, valid when the wavelength is much smaller than the length scale characteristic of the curvature. (In practice, this limitation need not be serious. E.g. the width of the Z^0 is not very sensitive to the Hubble constant H_0.)

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

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

may be written

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

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

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

where ϕ is a scalar transforming as

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

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

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

where $\mathcal{L} = \sqrt{g}\left(\frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - \frac{1}{2} m^2 \phi^2\right)$

or $$\frac{1}{\sqrt{g}} \partial_\mu \left(\sqrt{g}\, g^{\mu\nu} \partial_\nu \phi\right) + m^2 \phi = 0$$

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 $$\boxed{(\nabla_\mu \nabla^\mu + m^2)\, \phi = 0}$$

where covariant derivative ∇_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

It is the flat space KG eqn, with derivative replaced by covariant derivative.

To derive the identity, recall that for any matrix M

$$\ln\det(M+\delta M) = \operatorname{tr}\ln(M+\delta M)$$
$$= \operatorname{tr}\left[\ln M + \ln(\mathbb{1} + M^{-1}\delta M)\right]$$
$$= \operatorname{tr}\ln M + \operatorname{tr} M^{-1}\delta M$$

or
$$\frac{\delta(\det M)}{\det M} = \operatorname{tr} M^{-1}\delta M$$

$$\delta\sqrt{\det M} = \frac{1}{2}\sqrt{\det M}\,\operatorname{tr} M^{-1}\delta M$$

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
$$\Gamma^\lambda_{\mu\nu} = \frac{1}{2} g^{\lambda\sigma}\left[\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}\right]$$
$$\Rightarrow \Gamma^\lambda_{\lambda\nu} = \frac{1}{2} g^{\lambda\sigma}\left[\partial_\lambda g_{\nu\sigma} + \partial_\nu g_{\lambda\sigma} - \partial_\sigma g_{\lambda\nu}\right]$$

cancel

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

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 as a source in the Einstein equation.

If the action for gravity coupled to matter is

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

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

and we vary the metric

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

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

where
$$G^{\mu\nu} = R^{\mu\nu} - \tfrac{1}{2} g^{\mu\nu} R$$

We may now <u>define</u> a stress tensor by

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

then the eqn of motion is

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

— the Einstein equation

To derive $T^{\mu\nu}$ from

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

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

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

— which follows from $\delta M^{-1} = -M^{-1}\delta M M^{-1}$

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: general coord. invariance of $S_{matter} \Rightarrow \nabla_\nu T^{\mu\nu} = 0$

Now we want to construct a Hilbert space such that the fields acting on this space are causal. To do this, we'll make use of the solutions to the classical KG eqn., on which a natural "inner product" can be defined.

Let f, g be solutions to

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

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

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

where h_{ij} is the induced 3-metric on the surface Σ and n^μ is the forward-pointing unit normal to 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

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

– where V_μ is a 4-vector

(Remember that $\nabla^\mu V_\mu = \frac{1}{\sqrt{g}} \partial^\mu (\sqrt{g}\, V_\mu)$

– and that g reduces to h in an orthonormal coordinate system with $n^\mu = (1, 0, 0, 0)$.)

Hence

$$(f,g)_{\Sigma_1} - (f,g)_{\Sigma_2} = \int_{\Sigma_1 - \Sigma_2} d^3x \sqrt{h}\, n^\mu (f^* \partial_\mu g - \partial_\mu f^* g)$$

$$= \int_\Omega d^4x \sqrt{g}\, \nabla^\mu (f^* \nabla_\mu g - \nabla_\mu f^* g)$$

(where $\partial\Omega = \Sigma_1 - \Sigma_2$)

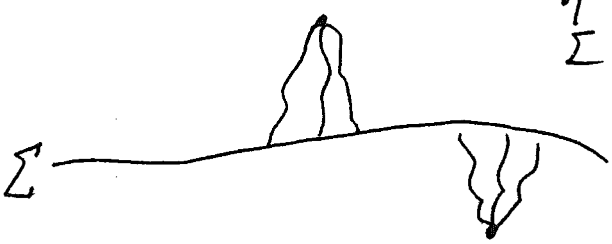
$= 0$ if f and g solve Klein-Gordon

— just as in the flat space case.

Remarks

- It is of course implicit in this construction that the Klein-Gordon equations has solutions that are globally defined in the 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 (without boundary) Σ such that no two points on Σ are connected by a time like 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 of this definition is that the physics 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 smooth such that $(\partial_\mu t)(\partial^\mu t) > 0$.)

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

$$\{\text{global solutions to KG eqn}\}$$
$$\simeq \{\text{initial data on a "time slice" } \Sigma\}$$

References

R. Wald "General Relativity", Chapter 8, 10
R. Geroch and G. Horowitz, "Global structure of spacetimes" in General Relativity: An Einstein centenary Survey" ed 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 actually holds more generally than a free field on a curved background, it applies to any coupling to external sources such that the field eqn for ϕ is linear and homogeneous (action S is quadratic). E.g. it applies to Klein-Gordon field coupled to 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

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

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

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

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

$$(\nabla^\mu \nabla_\mu + m^2) \phi = 0,$$

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 "back reaction" of the field ϕ on the geometry, 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 back reaction effects.

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

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

$$[\phi(x), \phi(y)]_{e.t.} = 0 = [\dot{\phi}(x), \dot{\phi}(y)]$$

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 Σ. Then

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

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

$$[n^\mu\partial_\mu\phi(x), n^\nu\partial_\nu\phi(y)]_\Sigma = 0$$

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

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 K-G eqn. To see this, we first show:

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

Thus, if ϕ satisfies the KG equation, we may use the slice independence of $(\ ,\ )_\Sigma$ to show.

- ϕ satisfies CCR on $\Sigma \iff \phi$ 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

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

and evaluate

$$[(f,\phi)_\Sigma,\ (g,\phi)_\Sigma\ ]$$

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

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

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

$$= -(f, g^*)_\Sigma$$

To see the if part, note that we can choose f, g and their normal derivatives to be arbitrary functions on Σ. From this initial data we obtain solutions to KG globally defined in spacetime, if 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 theory that we construct does not depend on how we slice the spacetime.

(ii) The theory is causal in the sense that

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

whenever there is a spacelike slice that contains both x and y

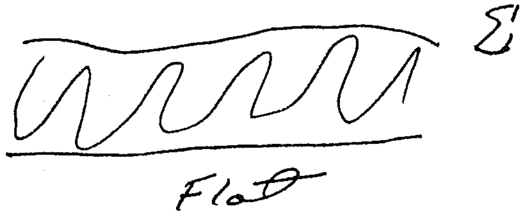
(For globally hyperbolic spacetimes, this slice presumably exists if there are no timelike or null curves connecting x and y.)

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 space theory, the construction of the Fock space does not require that the notion of a <u>particle</u> apply. We need only be able to divide the space of solutions of the KG eqn into subspaces with pos. def. and neg. def. KG norm.

The existence of a <u>complete</u> basis for the solutions to the KG eqn such that inner product on Σ satisfies

$$(u_i, u_j)_\Sigma = \delta_{ij}$$
$$(u_i, u_j^*)_\Sigma = 0$$
$$(u_i^*, u_j^*)_\Sigma = -\delta_{ij}$$

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 <u>discrete</u> 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 may 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 slice independent, and depends only on the solution and its first derivative at the slice.)

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

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

we have
$$(u_i, \phi) = a_i$$
$$-(u_i^*, \phi) = a_i^+$$
(evaluated on any slice)

Therefore, the CCR in the form

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

imply
$$(a_i, a_j) = -(u_i, u_j^*) = 0$$
$$(a_i^+, a_j^+) = 0$$
$$(a_i, a_j^+) = -(u_i, -u_j) = \delta_{ij}$$

– That is, the a_i, a_i^+ are conventionally normalized creation and annihilation operators

And since $[(f, \phi), (g, \phi)] = -(f, g^*)$ for a complete basis of solutions implies the CCR on any spacelike Σ, we could just as well assume the $a\ a^+$ commutators and then infer the canonical commutators that is, an alternative to canonical quantization is to choose a complete basis $\{u, u^*\}$ of solutions to KG, 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 construct the field ϕ on $\mathcal{H}$, which we have shown is local — i.e. satisfies $[\phi(x), \phi(y)] = 0$ if x and y lie 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. E.g. if u satisfies

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

then

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

satisfies

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

A linear combination of pos and neg norm solution is just as acceptable as u.

There is a natural way to decompose the space of solutions to the KG equation into subspaces on which the KG inner product is pos. def. and neg. def. respectively only in the special case of a <u>stationary</u> 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 <u>symmetry</u> 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, if $u(t,x)$ is a solution to the KG eqn, 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) <u>irreducible</u> representations. In other words, the operator

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

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

$$H u_K = \omega_K u_K$$
$$H u_K^* = -\omega_K u_K^*$$

— where ω_K is the frequency of the solution.

The solutions then have the form $u_K(t,x) = e^{-i\omega_K t}\sigma_K(\vec{x})$.

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

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

$$\Rightarrow \quad (\dot{f}, g) + (f, \dot{g}) = 0$$

So for solutions of definite frequency $\dot{u}_K = -i\omega_K u_K$ we have
$$i(\omega_K - \omega_j)\,(u_K, u_j) = 0$$

$\Rightarrow$ solution 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 pos. def for pos. freq. solutions, we have found a basis (the pos freq basis) such that
$$(u_i, u_j) = \delta_{ij}$$
$$(u_i, u_j^*) = 0$$
$$(u_i^*, u_j^*) = -\delta_{ij}$$

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

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

we have $\qquad [a_i, a_j^+] = \delta_{ij} \qquad [a_i, a_j] = 0$
$\qquad\qquad\qquad\qquad\qquad\qquad [a_i^+, a_j^+] = 0$

acting on Fock space

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

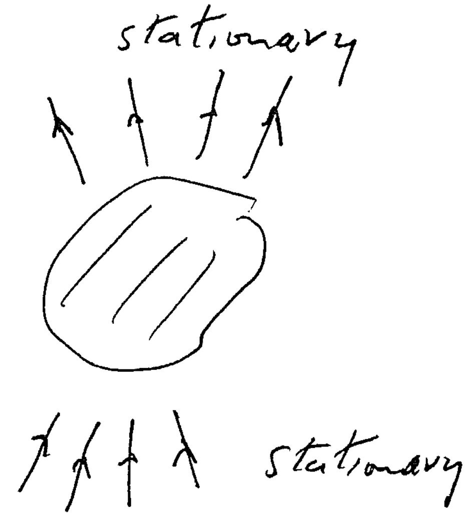
and the Hamiltonian H has the representation

$$H = \sum_K \omega_K a_K^+ a_K$$

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 will 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 over, and the Killing vector becomes spacelike.) In this case, the choice 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 of a spacetime that becomes asymptotically stationary in the past or future (or both).

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

$$p_i \to u_i \quad \text{in } \underline{\text{past}}.$$

Then $(p_i, p_j) = \delta_{ij}$ $(p_i, p_j^*) = 0$ $(p_i^*, p_j^*) = -\delta_{ij}$ 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

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

that becomes positive frequency in the future. These two bases need not coincide. A basis of positive freq solns in the past will propagate to a positive norm basis in the future, but not necessarily to a basis of positive frequency solns in the future. Hence, the incoming Fock space vacuum may evolve to a state that is not 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 outcoming particle state.

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

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

S will then be a unitary operator (it preserves the inner product – what comes in goes out).

Thus $|\psi_{out}\rangle = S^{-1}|\psi_{in}\rangle \Rightarrow \langle\psi_{out}| = \langle\psi_{in}|(S^{-1})^{+} = \langle\psi_{in}|S$

And we have

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

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

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

Remark:

We have defined S as a change of the Fock basis in the Hilbert space $\mathcal{H}$ of the theory.

$|\psi_{out}\rangle \in \mathcal{H}$ resembles $|\psi\rangle \in \mathcal{H}^{out}$ in future

$|\psi_{in}\rangle \in \mathcal{H}$ resembles $|\psi\rangle \in \mathcal{H}^{in}$ in past

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

An alternative is to define $\hat{S}: H_{in} \to H_{out}$ so that
$$|\psi_{in}\rangle = |\chi_{out}\rangle \Rightarrow \hat{S}|\psi\rangle = |\chi\rangle$$

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

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

and thus $$\langle j|\hat{S}|i\rangle = \langle j_{out}|S|i_{out}\rangle$$
$$= \langle j_{in}|S|i_{in}\rangle$$

In the language we have used here, we have
$$\phi = \sum_i (p_i a_i^{in} + p_i^* a_i^{in+}) = \sum_i (f_i a_i^{out} + f_i^* a_i^{out+})$$

(as on page (2.23)) where $\phi: \mathcal{H} \to \mathcal{H}$.

In the alternate language $\hat{a}^{in}: \mathcal{H}^{in} \to \mathcal{H}^{in}$

and $\hat{a}^{out}: \mathcal{H}^{out} \to \mathcal{H}^{out}$

These are related by
$$S\left[\sum_i (p_i a_i^{in} + p_i^* a_i^{in+})\right] S^{-1} = \sum_i (f_i a_i^{out} + f_i^* a_i^{out+})$$

and so
$$S(a^{in}\ a^{in+})S^{-1} = (a^{out}\ a^{out+})\begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$$

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

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

This is precisely the same equation that we have for S on page (2.27), provided we identify a^{in} and a^{out}.
In making the identification, we are recognizing the ~~natural~~ isomorphism $\mathcal{H}^{in} \to \mathcal{H}^{out}$, and that we must make use of this isomorphism to define S matrix elements (Since $\mathcal{H}^{in}$ and $\mathcal{H}^{out}$ are otherwise regarded as distinct spaces.)

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

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

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

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

If $\mathcal{O}^{in}$ is any operator, then

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

or

$$\mathcal{O}^{out} = S^{-1}\mathcal{O}^{in}S$$

- i.e. $S^{-1}\mathcal{O}^{in}S$ has the same matrix elements between out states as $\mathcal{O}^{in}$ does between in states.

We can calculate S if we can solve the KG eqn on the nontrivial BG. The solutions f, P solve the flat space eqn in past <u>and</u> future; since $\{u_i, u_i^*\}$ are a complete basis for solutions we have

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

for appropriate matrices α, β

Similarly,

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

But because the KG equation is linear and homogeneous everywhere the BG is nontrivial, we have

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

By expanding ϕ in terms of both bases, we find

$$\phi = \sum_i (p_i a_i^{in} + p_i^* a_i^{in+})$$
$$= \sum_j (f_j a_i^{out} + f_i^* a_i^{out+})$$

— and thus infer a linear relation among a^{in} a^{in+} and a^{out} a^{out+}. We may then solve for S by demanding

$$S^{-1} a^{in} S = a^{out}$$
$$S^{-1} a^{in+} S = a^{out+}$$

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 ϕ in terms of two different orthonormal bases for the KG solns (that are linearly related).

$$u_i' = \alpha_{ij} u_j + \beta_{ij} u_j^*$$
$$u_i'^* = \beta_{ij}^* u_j + \alpha_{ij}^* u_j^*$$

In matrix notation:

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

If both bases are normalized so that

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

then we have

$$\delta_{ij} = (u_i', u_j') = \alpha_{ik}^* \alpha_{jl} \delta_{kl} - \beta_{ik}^* \beta_{jl} \delta_{kl}$$
$$= (\alpha \alpha^+ - \beta \beta^+)_{ji}$$

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

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

left inverse $\rightarrow$ $$\begin{pmatrix} \alpha & \beta \\ \alpha^* & \beta^* \end{pmatrix}^{-1} = \begin{pmatrix} \alpha^+ & -\beta^T \\ -\beta^+ & \alpha^T \end{pmatrix}$$ (inverse is unique if it exists)

And therefore

(Thus a right inverse as well as left inverse $\Rightarrow$ additional identities on p 2.26)

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

Compare now the two mode expansions:

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

$$= \sum_i (u_i' a_i' + u_i'^* a_i^+)$$

$$= (a' \ a'^+) \begin{pmatrix} u' \\ u'^* \end{pmatrix}$$

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

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

$$(a' \ a'^+) \begin{pmatrix} u' \\ u'^* \end{pmatrix} = (a \ a^+) \begin{pmatrix} \alpha^+ & -\beta^T \\ -\beta^+ & \alpha^T \end{pmatrix} \begin{pmatrix} u' \\ u'^* \end{pmatrix}$$

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

$$(a \ a^+) = (a' \ a'^+) \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$$

$$(a' \ a'^+) = (a \ a^+) \begin{pmatrix} \alpha^+ & -\beta^T \\ -\beta^+ & \alpha^T \end{pmatrix}$$

and taking transposes

$$\boxed{\begin{pmatrix} a' \\ a'^+ \end{pmatrix} = \begin{pmatrix} \alpha^* & -\beta^* \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} a \\ a^+ \end{pmatrix}, \quad \begin{pmatrix} a \\ a^+ \end{pmatrix} = \begin{pmatrix} \alpha^T & \beta^+ \\ \beta^T & \alpha^+ \end{pmatrix} \begin{pmatrix} a' \\ a'^+ \end{pmatrix}}$$

Since
$$\begin{pmatrix} \alpha^T & \beta^\dagger \\ \beta^T & \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \alpha^* & -\beta^* \\ -\beta & \alpha \end{pmatrix}^{-1},$$
we have the additional identities
$$\boxed{\begin{aligned} \alpha^T\alpha^* - \beta^\dagger\beta &= \mathbb{1} \\ \alpha^\dagger\beta^* - \beta^\dagger\alpha &= 0 \end{aligned}}$$

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

For $\beta \neq 0$, we have changed the positive norm subspace of the space of solutions to KG. 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 ∞ number of degrees of freedom, this is true only subject to certain conditions that will emerge from the calculation below.)

As described on page 2.21, we may define a unitary change of basis by

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

in which case

$$U^{-1} a U = a'$$
$$U^{-1} a^{+} U = a'^{+}$$

(Note: U will be unitary if it preserves the norm of $|0'\rangle$ – then, since it preserves commutators, it preserves normal all Fock states.

From these equations and the Bogolubov transformation, we can solve for U in terms of a or 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^{+}

$$U = \; :U(a, a^{+}):$$

(where double dots denote normal ordering). Normal-ordered means that all a's lie to the right of all a^{+}'s. To solve

$$aU = Ua' = U(\alpha^{*} a - \beta^{*} a^{+}),$$
$$a^{+} U = Ua'^{+} = U(-\beta a + \alpha a^{+}),$$

we note that operators a, a^{+} act on normal-ordered functions as

$$a_i :\mathcal{O}: \; = \; :\left(a_i + \frac{\partial}{\partial a_i^{+}}\right)\mathcal{O}:$$
$$a_i^{+} :\mathcal{O}: \; = \; :a_i^{+}\mathcal{O}:$$
$$:\mathcal{O}: a_i \; = \; :a_i \mathcal{O}:$$
$$:\mathcal{O}: a_i^{+} \; = \; :\left(a_i^{+} + \frac{\partial}{\partial a_i}\right)\mathcal{O}:,$$

since $\qquad [a_i, f(a^\dagger)] = \frac{\partial}{\partial a_i^\dagger} f(a^\dagger)$

$\qquad\qquad [f(a), a_i^\dagger] = \frac{\partial}{\partial a_i} f(a)$

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

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

$$(ii) \quad a^\dagger\, U = \left[-\beta a + \alpha\left(a^\dagger + \frac{\partial}{\partial a}\right)\right] U$$

(normal ordering now understood and not explicitly indicated).

We solve this by means of the Ansatz

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

$$= C \exp\left[\tfrac{1}{2}\left(a M_{11} a + a M_{12} a^\dagger + a^\dagger M_{21} a + a^\dagger M_{22} a^\dagger\right)\right]$$

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

$$\frac{\partial}{\partial a} U = (M_{11} a + M_{12} a^\dagger)\, U,$$

$$\frac{\partial}{\partial a^\dagger} U = (M_{21} a + M_{22} a^\dagger)\, U,$$

and we have the algebraic equations:

$$(i)\quad (a + M_{21} a + M_{22} a^{+}) = \alpha^{*} a - \beta^{*}(a^{+} + M_{11} a + M_{12} a^{+})$$

$$(ii)\quad a^{+} = -\beta a + \alpha(a^{+} + M_{11} a + M_{12} a^{+})$$

Since the coefficients of a and a^{+} must vanish (ii) implies

$$\begin{aligned} \mathbb{1} &= \alpha + \alpha M_{12} \\ 0 &= -\beta + \alpha M_{11} \end{aligned} \Longrightarrow \boxed{\begin{aligned} M_{12} &= \alpha^{-1} - \mathbb{1}, \\ M_{11} &= \alpha^{-1}\beta \end{aligned}}$$

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

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

which shows that $\alpha\alpha^{+}$ has no zero eigenvalue. Thus $\langle\psi|\alpha\alpha^{+}|\psi\rangle = \|\alpha^{+}|\psi\rangle\|^{2} > 0$; α^{+} has trivial kernel, and therefore the range of α is the whole space. Furthermore

$$(\alpha^{+}\alpha)^{*} = \mathbb{1} + \beta^{+}\beta \quad \text{shows that}$$

Kernel $\alpha = 0$ -- so α has a left and right inverse.

From (i) we find

$$M_{22} = -\beta^{*} - \beta^{*} M_{12} = -\beta^{*}\alpha^{-1}$$

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

~~And last equation was satisfied because of the identity~~

or
$$\boxed{\begin{aligned} M_{22} &= -\beta^* \alpha^{-1}, \\ M_{21} &= -\mathbb{1} + \alpha^* - \beta^* \alpha^{-1} \beta \end{aligned}}$$

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...

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

E.g., from
$\beta\alpha^T = \alpha\beta^T$ we have $\alpha^{-1}\beta = \beta^T(\alpha^T)^{-1} = (\alpha^{-1}\beta)^T$

$$\beta^\dagger\alpha = \alpha^T\beta^* \Rightarrow \beta^*\alpha^{-1} = (\alpha^T)^{-1}\beta^\dagger = (\beta^*\alpha^{-1})^T$$

and from
$$\mathbb{1} = \alpha^T\alpha^* - \beta^\dagger\beta = \alpha^T\alpha^* - (\alpha^T\beta^*\alpha^{-1})\beta,$$
we have
$$(\alpha^T)^{-1} = \alpha^* - \beta^*\alpha^{-1}\beta,$$
so that $M_{12}^T = M_{21}$

We have now found

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

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

$$|0'\rangle = U^{+}|0\rangle \Rightarrow \langle 0'|0'\rangle = \langle 0|0\rangle = \mathbb{1}$$

where $|0\rangle$ is the vacuum satisfying $a_i|0\rangle = 0$

Since the adjoint of a normal ordered operator is normal-ordered, we have

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

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

Now, we invoke the identity

$$\langle 0| \exp\left(\tfrac{1}{2} a M a\right) \exp\left(\tfrac{1}{2} a^{+} M^{*} a^{+}\right)|0\rangle$$

$$= \left[\det\left(\mathbb{1} - M M^{*}\right)\right]^{-\frac{1}{2}}, \text{ where } M = M^{T}$$

(We'll return to the derivation of the identity shortly.)

Thus

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

We can simplify the determinant by recalling the identities

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

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

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

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

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

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

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

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

It has the same form when expressed in terms of a^{out}, $a^{out\dagger}$, since

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

We have

$$|\langle 0\,\mathrm{out}|0\,\mathrm{in}\rangle|^2 = (\det \alpha^\dagger\alpha)^{-\frac{1}{2}}$$

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

$$N_i = \langle 0\,\mathrm{in}|\underbrace{a_i^{\mathrm{out}\dagger} a_i^{\mathrm{out}}}_{\text{not summed}}|0\,\mathrm{in}\rangle$$

$$\langle 0\,\mathrm{in}|(-\beta_{ij}\, a_j^{\mathrm{in}})(-\beta^*_{ik}\, a_k^{\mathrm{in}\dagger})|0\,\mathrm{in}\rangle$$

$$= (\beta\beta^\dagger)_{ii} = \sum_j |\beta_{ij}|^2$$

— 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 total number of particles produced is

$$N = \sum_i N_i = \mathrm{tr}(\beta\beta^\dagger)$$

And since $\alpha\alpha^\dagger = \mathbb{1} + \beta\beta^\dagger$, the condition that

$$\det(\alpha\alpha^\dagger) = \det(\mathbb{1} + \beta\beta^\dagger) < \infty$$

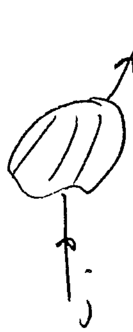
is precisely $N < \infty$

the canonical transformation
$$(a^{in}, a^{in\dagger}) \to (a^{out}, a^{out\dagger})$$
cannot be implemented by a unitary operator if the $|0_{in}\rangle$ 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 are produced by the fluctuating geometry. It does not happen if the (smooth) spacetime is flat outside a compact region, for ~~fluctuating~~ geometry in a compact region does not produce arbitrarily soft particles (a theorem of R. Wald, Ann. Phys. 118 (1979) 490, "Existence of the S-matrix in QFT in Curved Spacetime").)

Some other S-matrix elements are:

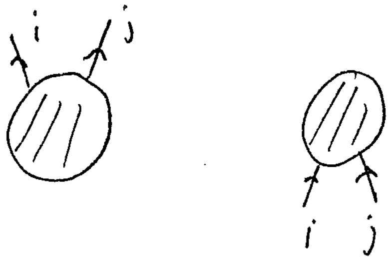
$$\langle i\,out | j\,in\rangle = \langle 0_{out}|0_{in}\rangle \left(\mathbb{1} + \underbrace{\alpha^{-1} - \mathbb{1}}_{\text{"connected" part}}\right)_{ij} = \alpha^{-1}_{ij}$$



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

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

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



Particles are created or annihilated only if $\beta \neq 0$ (Bogolubov transformation mixes pos. and neg 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 would 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 $\rightarrow$ many-particle amplitudes. Consider for example

$$\langle i_1 - i_{2n} \text{ out} | 0 \text{ in}\rangle$$

$$= \langle i_1 \cdots i_{2n} | S | 0 \rangle = \langle i_1 \cdots i_{2n} | \tfrac{1}{n!}(\tfrac{1}{2} a^\dagger V a^\dagger)^n | 0 \rangle$$

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

Allowing the $2n$ $a^\dagger$'s to annihilate (to the left) the $2n$ particles $i_1 \cdots i_{2n}$ generates $(2n)!$ terms, each term giving a product

$V_{..} V_{..} \cdots V_{..}$ of n matrix elements of 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 the indices that leave the pairing unchanged.

Thus the $\frac{1}{n!2^n}$ gets cancelled, and we have

$$\langle i_1 \cdots i_{2n} \text{ out} \,|\, 0 \text{ in} \rangle$$

$$= V_{i_1,i_2} V_{i_3,i_4} \cdots V_{i_{2n-1},i_{2n}} + \text{all other pairings,}$$

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

E.g.

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

We return now to the derivation of the identity

$$\langle 0 | \exp\left(\tfrac{1}{2} a M a\right) \exp\left(\tfrac{1}{2} a^\dagger M^* a^\dagger\right) | 0 \rangle$$

$$= \left[\det(\mathbb{1} - M M^*)\right]^{-\frac{1}{2}} \quad (\text{where } M = M^T).$$

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 $|0\rangle$

$$|\psi\rangle = \psi(a^\dagger)|0\rangle \equiv \sum_{n=0}^{\infty} \sum_{i_1 \cdots i_n} \underset{\Sigma\,(\text{symmetric})}{\psi^{(n)}_{i_1 \cdots i_n}} a^\dagger_{i_1} \cdots a^\dagger_{i_n} |0\rangle$$

Claim:

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

Here, on the RHS, a_i a_i^+ are complex c-nos and

$$\int da\,da^+ \equiv \int \prod_i da_i\,da_i^+$$ is an integral $\int_{-\infty}^{\infty}$ over real and imaginary part of each a_i

we see that, to verify the claim, it is enough to show (since we can expand in powers of a^+):

$$\langle 0 | a_{i_1} \cdots a_{i_n} a_{j_1}^+ \cdots a_{j_m}^+ | 0 \rangle$$

$$= \frac{\int da\,da^+ \; a_{i_1} \cdots a_{i_n} a_{j_1}^+ \cdots a_{j_m}^+ e^{-a^+ a}}{\int da\,da^+ \; e^{-a^+ a}}$$

We can derive this identity by evaluating both sides.

Commuting a's through a^+'s, we find

$$\langle 0 | a_{i_1} \cdots a_{i_n} a_{j_1}^+ \cdots a_{j_m}^+ | 0 \rangle = 0 \quad (m \neq n)$$

$$= \delta_{i_1 j_1} \cdots \delta_{i_n j_n} + \text{perms } (n! \text{ Terms altogether}) \quad (m = n)$$

To evaluate integral on LHS, construct the generating function

$$Z[J] = \int da\,da^+ \, e^{\bar{J} a} e^{a^+ J} e^{-a^+ a}$$

We complete the square:

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

shift the integral:

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

Now

$$\int da\,da^\dagger\, a_{i_1} \cdots a_{i_n} a^\dagger_{j_1} \cdots a^\dagger_{j_m} e^{-a^\dagger a} \Big/ \int da\,da^\dagger e^{-a^\dagger a}$$

$$= \frac{1}{Z[0]} \frac{\partial}{\partial \bar{J}_{i_1}} \cdots \frac{\partial}{\partial \bar{J}_{i_n}} \frac{\partial}{\partial J_{j_1}} \cdots \frac{\partial}{\partial J_{j_m}} Z[J] \Big|_{J = \bar{J} = 0}$$

$$= \frac{\partial}{\partial \bar{J}_{i_1}} \cdots \frac{\partial}{\partial J_{j_m}} e^{\bar{J}J} \Big|_{J = \bar{J} = 0}$$

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

$$= \frac{\partial}{\partial J_{j_1}} \cdots \frac{\partial}{\partial J_{j_n}} (J_{i_1} \cdots J_{i_n})$$

$$= \delta_{i_1 j_1} \cdots \delta_{i_n j_n} + \text{perms}$$

By means of this trick, we have

$$\langle 0 | \exp\left(\tfrac{1}{2} a M a\right) \exp\left(\tfrac{1}{2} a^\dagger M^* a^\dagger\right) | 0 \rangle$$

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

You can evaluate such an integral by changing variables to real

$$X = \frac{1}{\sqrt{2}}(a + a^\dagger) \qquad Y = \frac{1}{i\sqrt{2}}(a - a^\dagger)$$

A real Gaussian integral

$$\int dX \, e^{-\frac{1}{2} X A X} \qquad (A = A^T)$$

may be evaluated if A has an orthonormal basis of eigenvectors

$$A e_n = \lambda_n e_n$$

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

$$\frac{\int dX \, e^{-\frac{1}{2} X \cdot A X}}{\int dX \, e^{-\frac{1}{2} X \cdot X}} = \prod_n \left[\frac{\int dX_n e^{-\frac{1}{2} X_n \lambda_n X_n}}{\int dX_n \, e^{-\frac{1}{2} X_n^2}} \right]$$

$$= \prod_n \lambda_n^{-\frac{1}{2}} = (\det A)^{-\frac{1}{2}}$$

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

Writing our integral in terms of real variables and using elementary properties of determinants, we find (exercise)

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

and

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

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

— which was to be shown.