The S-matrix and time-ordered products

We will now begin to work on a methodology for calculating the matrix elements $M$ that appear in cross sections and decay rates given some underlying Lagrangian description. As we have hinted at before, there is a relationship between correlation functions of quantum fields and $S$-matrix elements. In particular, the $S$-matrix elements correspond to non-trivial complex structure in the vacuum expectation values of products of fields. In particular, as we will soon see, $S$-matrix elements are given by

$$\langle f | S | i \rangle = \left[ i \int d^4x_1 e^{-ip_1x_1} \left( \Box + m^2 \right) \right] \cdots \left[ i \int d^4x_n e^{ip_nx_n} \left( \Box + m^2 \right) \right] \times \langle \Omega | T \{ \phi(x_1) \cdots \phi(x_n) \} | \Omega \rangle$$

(172)

where $| \Omega \rangle$ is the ground state, and $\phi$ is the interacting field. This formula is called the LSZ (Lehmann-Symanzik-Zimmerman) Reduction Formula. The integrals over the operators acting on the vacuum expectation values serve to project that function onto its poles (which in turn correspond to asymptotic states appearing in the definition of the $S$-matrix).

Note that the $S$-matrix elements then only encode a tiny (although crucially important) amount of info that is available in a typical correlation function.

The LSZ reduction formula is proved by utilizing the asymptotic properties of the field $\phi$, which can be expressed in terms of annihilation and creation operators as

$$\phi(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \left[ a_p(t)e^{-ipx} + a_p^\dagger(t)e^{ipx} \right]$$

(173)

where the time dependence of the annihilation and creation operators is non-trivial if the theory contains interactions.

The crucial identity required relates the operators acting on the fields $\phi$ to the annihilation and creation operators evaluated at the far boundaries of time:

$$i \int d^4x e^{ipx} \left[ \Box + m^2 \right] \phi(x) = \sqrt{2\omega_p} \left[ a_p(\infty) - a_p(-\infty) \right]$$

(174)

Note we mean the true vacuum of the full theory with interactions/nonlinearities. In this case, each ground state of each mode is slightly perturbed (assuming small interactions/non-linearities) from the original non-interacting theory ground state, with a net effect that the interacting ground state is “far removed” from the non-interacting ground state. By $\phi$, we mean the operator that solves the full interaction equations of motion, not the solution we worked out for non-interacting scalar fields.

By and large, the most important information is contained in the poles and branch cuts that live in these correlation functions, so it is not some storehouse of info of mythical proportions, as one might be tempted to believe given the words used in the text. There is also redundancy, where cuts in lower point correlators correspond to poles in higher point correlators - this redundancy is encoded in equations referred to as the Schwinger-Dyson relations.

A motivation for the $a^\dagger$’s creating single particle states is that the spectrum can be gapped if there is a mass term for $\phi$. The spectrum of eigenvalues of the Hamiltonian contains typically a set of single particle states that are separated from multi-particle continua in the $E - |\beta|$ plane.
I will not reproduce the proof of this identity, which you can find in the text (or similar versions in other texts). I will note, however, that there is one important assumption that is made: the **theory is free at early and late times**.\(^{56}\)

Now the \(S\)-matrix is the time evolution operator evaluated at large times - If the \(a\)'s and \(a^\dagger\)'s create single particle states at some reference time \(t_0\), then we have that \( |i\rangle = \sqrt{2\omega_{p_1}2\omega_{p_2} a_{p_1}^\dagger (t_0) a_{p_2}^\dagger (t_0)} |\Omega\rangle\) and \( \langle f| = \langle \Omega| \sqrt{2\omega_{k_1} \cdots 2\omega_{k_n}} a_{k_1} (t_0) \cdots a_{k_n} (t_0) \), and the \(S\)-matrix is then

\[
\langle f | S | i \rangle = \frac{\sqrt{2\omega_{p_1}2\omega_{p_2}2\omega_{k_1} \cdots 2\omega_{k_n}}}{\sqrt{2\omega_{p_1}2\omega_{p_2}2\omega_{k_1} \cdots 2\omega_{k_n}}} \langle \Omega| a_{k_1} (\infty) \cdots a_{k_n} (\infty) a_{p_1}^\dagger (\infty) a_{p_2}^\dagger (\infty) | \Omega \rangle \\
\times \langle \Omega | T \left\{ [a_{k_1} (\infty) - a_{k_1} (-\infty)] \cdots [a_{k_n} (\infty) - a_{k_n} (-\infty)] [a_{p_1}^\dagger (\infty) - a_{p_1}^\dagger (-\infty)] [a_{p_2}^\dagger (\infty) - a_{p_2}^\dagger (-\infty)] \right\} | \Omega \rangle
\] (175)

So we see that by proving the above relationship for the \(\phi\) fields, we can show that the LSZ reduction formula holds so long as we can isolate the interactions from the boundary.\(^{57}\)

**The power of LSZ**

In our discussion, we restricted ourselves to projecting out the singularities (poles) associated with the single particle asymptotic states created by the quantum fields \(\phi\). However, the spectrum of states in an interacting theory can be far richer. This is the case already when looking at the two point function in an interacting theory. In this case, the interactions of a theory can modify the mass \(m\), or the normalization of the states - the difference between the \(a\)'s of an interacting theory and those of a “corresponding” non-interacting one can be far different. This is only the simple two-point - there are far more complicated operators one might consider that still create single particle states. For example, one might consider bound states: in QED, electrons and positrons can pair together to create semi-stable “atoms” made from electrons and their antiparticles. The LSZ reduction formula can project out these states as well, so long as you know how to write an operator that has some overlap with the quantum field that creates such a bound-state.

**The Feynman Propagator**

Recall that in classical field theory, and in old fashioned perturbation theory, we needed to use Green’s functions to propagate the fields
from some sources to some points at which classical correlators could be measured. We now need the analog for quantum field theory - a way to calculate the time-ordered product of fields that appears in the LSZ reduction formula.\footnote{These $n$-point correlators are the $n$-point Green’s functions.} In classical perturbation theory, an arbitrarily precise expression for the solution to a non-linear equation of motion involved using the classical propagator to stitch together vertices with sources and an endpoint (where the field would be measured). In old fashioned perturbation theory, the process was somewhat clunky, with advanced and retarded Green’s functions being used for different cases for whether it was one electron or the other acting as the source.

Here we will derive a propagator for scalar quantum field theory that by-passes such technicalities, and streamlines the process of computing various $n$-point correlators by building them out of vertices and propagators (or two point correlation functions).

To derive the Feynman propagator, it is sufficient to consider a free scalar field theory. Recall the definition of the field (where the annihilation/creation operators are now time-independent):

$$\phi_0(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2\omega_k}} \left[ a_k e^{-ikx} + a_k^\dagger e^{ikx} \right]$$  \hspace{1cm} (176)

where for the free theory we can use the relativistic energy-momentum relation $k^0 = \sqrt{m^2 + |k|^2}$. As was the case before, we label the non-interacting vacuum state as $|0\rangle$, and we can then easily work out the vacuum expectation value of the product of two scalar fields evaluated at different space-time coordinates:

$$\langle 0 | \phi_0(x_1) \phi_0(x_2) | 0 \rangle = \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} \frac{1}{\sqrt{2\omega_{k_1}}} \frac{1}{\sqrt{2\omega_{k_2}}} \langle 0 | a_{k_1} a_{k_2}^\dagger | 0 \rangle e^{-ik_1 x_1 + ik_2 x_2}$$  \hspace{1cm} (177)

Using our normalization for the annihilation and creation operators, the matrix element in the above expression gives a simple delta function: $(2\pi)^3\delta^3(k_1 - k_2)$. Thus we find

$$\langle 0 | \phi_0(x_1) \phi_0(x_2) | 0 \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} e^{-ik(x_1 - x_2)}$$  \hspace{1cm} (178)

In the end, we will be interested in the vacuum expectation value for time ordered products of fields, so using the above expression, we can write:

$$\langle 0 | T \{ \phi_0(x_1) \phi_0(x_2) \} | 0 \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} e^{-ik(x_1 - x_2)} \Theta(t_1 - t_2) + \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} e^{ik(x_1 - x_2)} \Theta(t_2 - t_1)$$

$$= \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} e^{-ik(x_1 - x_2)} \left[ e^{-i\omega_k \tau} \Theta(\tau) + e^{i\omega_k \tau} \Theta(-\tau) \right]$$  \hspace{1cm} (179)
where in the last line we have used $\tau \equiv t_1 - t_2$. Note that the time ordering decides for you whether to use the retarded or advanced propagator automatically.

Now, as you showed in your homework, you can write the Heaviside function in terms of a Fourier transform, and the result leads to

$$e^{-i\omega t} \Theta(t) + e^{i\omega t} \Theta(-t) = \lim_{\epsilon \to 0} \frac{-2\omega_k}{2\pi i} \int_{-\infty}^{\infty} \frac{d\omega}{\omega^2 - \omega_k^2 + i\epsilon} e^{i\omega t}$$  \hspace{1cm} (180)

To prove this identity, you can examine the structure of the function in terms of its singularities in the complex plane. There are two poles associated with the integrand: one at $\omega = \omega_k - i\epsilon$, and the other at $\omega = -\omega_k + i\epsilon$. Depending on the sign of $\tau$, you evaluate the integral by completing the contour either above (for $\tau > 0$), or below (for $\tau < 0$), and enclosing either the latter or the former of the two poles. Application of the residue theorem (remembering the minus sign associated with closing the contour in the CW direction for $\tau < 0$) leads to the equality shown.

We can now combine these results to write the final expression for the VEV of the time-ordered product of two free scalar fields (aka the **Feynman propagator**):

$$D_F(x_1 - x_2) \equiv \langle 0 | T \{ \phi_0(x_1) \phi_0(x_2) \} | 0 \rangle$$  

$$= \lim_{\epsilon \to 0} \int \frac{d^4k}{(2\pi)^4} \frac{i}{k^2 - m^2 + i\epsilon} e^{ik(x_1 - x_2)}$$  \hspace{1cm} (181)

Note that in replacing the Heaviside functions with integrals over $\omega$ we have broken the relationship between the energy and 3-momenta that is present in the definition of the quantum fields. In calculating scattering amplitudes using these propagators, this will make it appear as though there are intermediate “particles” that do not satisfy the on-shell condition. These have gained the name “virtual” particles. Of course, their appearance in amplitudes has more to do with a simplification of the algorithm for calculating amplitudes than it does with real physics.60

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60 This step is crucial in defining the Feynman propagator. You will often hear the "i$\epsilon$" trick referred to in the process of calculating matrix elements in quantum field theory. It is this $i\epsilon$-trick that handles automatically and efficiently the arrangements of retarded and advanced propagators that appear as intermediate steps in some complicated calculation for getting some quantum mechanical amplitude.

61 The power in using this formalism is that it is far simpler to keep track of Lorentz invariance using this formalism. The expression for the Feynman propagator is manifestly Lorentz invariant, and in perturbation theory, its use will be associated with a 4-momentum conservation that is manifest at each vertex corresponding to an insertion of the coupling between the fields.