Green's Functions and S Matrices from the Operator (Hamiltonian) Viewpoint

1 Field Theory in a Box

Consider a real scalar field, with lagrangian

$$\mathcal{L} = -\frac{1}{2} (\partial_\mu \phi)^2 - m^2 \phi^2. \tag{1}$$

This is solved by

$$\phi(\vec{x},t) = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \frac{1}{\sqrt{2\omega(k)}} [a(\vec{k})e^{ik\cdot x} + a^{\dagger}(\vec{k})e^{-ik\cdot x}].$$
(2)

Imposing canonical commutation relations on $\phi, \dot{\phi}$, gives

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

 $N(\vec{k})=a^{\dagger}(\vec{k})a(\vec{k})$ is a conventionally normalized number operator.

2 Pictures in Quantum Mechanics

In 217, you did a problem (chapter 9 of Srednicki) developing perturbation theory in the interaction picture. This handout is meant as a short review.

We usually work with quantum mechanics in the Schrödinger picture, in which states depend on time, but operators like x and p are independent of time. In the Schrödinger picture:

$$|\Psi_S(t)\rangle = U(t, t_o)|\Psi(t_o)\rangle.$$
(4)

The time-development operator is just:

$$U(t, t_o) = e^{-iH(t-t_o)} \tag{5}$$

and it satisfies:

$$i\frac{\partial}{\partial t}U = HU.$$
(6)

It has the important properties that:

$$U^{\dagger}(t,t_o) = U(t_o,t); U(t,t_1)U(t_1,t_o) = U(t,t_o)$$
(7)

Another picture which is convenient for certain purposes is the Heisenberg picture. In this picture, the states are independent of time, but operators are now time-dependent:

$$|\Psi_H(t)\rangle = U^{\dagger}(t, t_o)|\Psi_S(t)\rangle = |\Psi_S(t_o)\rangle$$
(8)

while

$$\mathcal{O}_H(t) = U^{\dagger}(t, t_o) \mathcal{O}_{\mathcal{S}} U(t, t_o).$$
(9)

Note that with this definition:

$$<\Psi_H |\mathcal{O}_H|\Psi_H> = <\Psi_S |\mathcal{O}_S|\Psi_S>$$
 (10)

and

$$i\frac{\partial}{\partial t}\mathcal{O}_H = -U^{\dagger}H\mathcal{O}_S U + U^{\dagger}\mathcal{O}_S HU = -[H,\mathcal{O}_H]$$
(11)

This is actually an operator version of Ehrnfest's theorem. You can check, for example, that for a particle in a potential, the *operators* obey the classical equations of motion.

Probably the most useful picture is the "interaction picture." Here we suppose that the Hamiltonian is of the form:

$$H = H_o + H_I \tag{12}$$

where H_o is a Hamiltonian which we know how to diagonalize (in the field theory case, this will be the free Hamiltonian).

Then we write

$$|\Psi_I\rangle = e^{iH_o(t-t_o)}|\Psi_S(t)\rangle = e^{iH_o(t-t_o)}e^{-iH(t-t_o)}|\Psi_S(t_0)\rangle$$
(13)

So we define the time-development operator in the interaction picture:

$$U_I(t, t_o) = e^{iH_o(t-t_o)}e^{-iH(t-t_o)}$$
(14)

and define the time-dependent operators:

$$\mathcal{O}_I = e^{iH_o(t-t_o)} \mathcal{O}_S e^{-iH_o(t-t_o)} \tag{15}$$

Then it is a simple exercise to show that U_I obeys:

$$i\frac{\partial}{\partial t}U_I = H_I U_I; U(t,t) = 1.$$
(16)

 U_I has composition properties similar to those of U. These are most easily proven by writing U in a slightly different form:

$$U_I(t,t') = e^{iH_o(t-t_o)} e^{-iH(t-t')} e^{-iH_o(t'-t_o)}$$
(17)

This obeys the correct equation and boundary condition (check!). It also manifestly satisfies:

$$U_I^{\dagger}(t, t_o) = U_I(t_o, t); U_I(t, t_1)U_I(t_1, t_2) = U(t, t_2)$$
(18)

Solving this equation iteratively (see your favorite quantum mechanics book or exercise 9.3 in Srednicki) yields the standard expansion of time-dependent perturbation theory.

$$U_I = T e^{-i \int d^4 x \mathcal{H}_I(x)}.$$
(19)

Time ordering is useful because it is a Lorentz invariant notion.

3 Green's functions

Correlation functions are given by

$$\langle \Omega | T\phi(x_1) \dots \phi(x_n) | \Omega \rangle = \frac{\langle 0 | T\phi_I(x_1) \dots \phi_I(x_n) e^{-i \int d^4 x \mathcal{H}_I(x)} | 0 \rangle}{\langle 0 | Te^{-i \int d^4 x \mathcal{H}_I(x)} | 0 \rangle}$$
(20)

where $|\Omega\rangle$ is the exact ground state of the field theory. Green's functions can now be evaluated by Wick's theorem, giving the same expansion as obtained from the path integral.

4 The S Matrix

4.1 Born Approximation in Quantum Mechanics

The proper derivation of the formulae for the S-matrix considers wave packets . But if one is willing to forget such niceties, one can derive the usual expressions very quickly.

First, in non-relativistic scattering, we are interested in

$$<\vec{p}_f|U_I(T,-T)|\vec{p}_I>,$$

where it is understood that in the end we want to take the limit $T \to \infty$. To first order, staying away from the forward direction (so that the unit operator piece in U does not contribute, this is

$$<\vec{p}_{f}|U_{I}(T,-T)|\vec{p}_{I}> = <\vec{p}_{f}|\int_{-T}^{T}dt e^{-i(E_{f}-E_{i})t}V|\vec{p}_{I}>$$

= $2\pi\delta(E_{f}-E_{i})<\vec{p}_{f}|V|\vec{p}_{I}>.$

So far this is ok. Now comes the sleight of hand. We need to square this. Interpret

$$\delta(E_f - E_i)^2 = \delta(0)\delta(E_f - E_i)$$
$$\delta(0) = \lim_{T \to \infty} \frac{1}{2\pi} \int_{-T}^{T} dt$$
$$= \frac{1}{2\pi} T.$$

To get the cross section, divide by T, to get the transition rate per unit time, and integrate over final states (e.g. all momenta in some solid angle, $\Delta\Omega$), and divide by the flux, $\frac{p}{m}$, to give

$$d\sigma = \int_{\Delta\Omega} \frac{d^3 p_f}{(2\pi)^3} |\langle \vec{p}_f | V | \vec{p}_i \rangle |^2 \frac{m}{p} \delta(E_f - E_i)$$

This is the famous Born approximation for the scattering by a particle in a potential.

4.2 Relativistic Generalization

Now we repeat this for field theory. We specialize to processes with two incoming particles, and any number of outgoing particles. So we are interested in

$$< p_1 \dots p_N | U(T, -T) | k_A k_B > = < p_1 \dots p_N | S | k_A k_B >$$

(technically, the S matrix is defined to act between in and out states; see your text). Then we define:

$$S = 1 + iT$$

Because of space-time translation invariance, the T matrix always contains a δ function, so we write:

$$< p_1 \dots p_N |iT| k_A k_B >= (2\pi)^4 \delta(k_A + k_B - \sum_{i=1}^{n} p_i) i\mathcal{M}(k_A, k_B \to \{p_i\})$$

Note here that all momenta are "on shell", $\vec{p}_i^2 + m^2 = E_i^2$.

Now we square. We interpret $\delta(0) = VT$, in analogy to what we did in the non-relativistic case. Divide now by T, to get the transition rate per unit time, and V, corresponding to a constant target density (non-localized states). Divide also by the flux, which as in the non-relativistic limit goes as $|v_A - v_B|$, but is also multiplied by $2E_A 2E_B$ due to our normalization of the states. You can check that this flux is invariant under boosts along the beam axis. So we have:

$$d\sigma = \frac{1}{2E_A \ 2E_B |v_A - v_B|} \int \Pi\left(\frac{d^3 p_i}{(2\pi^3)}\right) \frac{1}{2E_{p_i}} |\mathcal{M}(k_A, k_B \to \{p_i\})|^2 (2\pi)^4 \delta(k_A + k_B - \sum p_i).$$

Exercise: Repeat this exercise for the decay of a particle.

4.3 Perturbative Expansion for the S matrix

Now we can evaluate the S matrix, using our formula above. To lowest order in couplings, the initial and final states are simple. For ϕ_I , we can write:

$$\phi_I(x) = \int \frac{d^3k}{2\sqrt{\omega(k)}(2\pi)^3} [a_I(\vec{k})e^{ik\cdot x} + a_I^{\dagger}(\vec{k})e^{-ik\cdot x}]$$
(21)

then, in the limit of zero interaction, the *a*'s and a^{\dagger} 's create and annihilate the momentum states. When we expand $e^{-i\mathcal{H}}$, we can take powers of ϕ to annihilate the creation and annihilation operators to the far left and far right, and use Wick's theorem to eliminate the rest. More precisely, we can use Wick's theorem in a slightly more general form than presented in chapter 8 – directly in terms of operators. Then the result is immediate. In order to understand this more general form of Wick's theorem, one needs to define an object known as the "normal product". Basically,

$$N(\phi(x_1)\cdots\phi(x_n)) \tag{22}$$

is an object with all annihilation operators to the right, all creation operators to the left. Wick's theorem then asserts that

$$T(\phi(x_1)\dots\phi(x_n)) = ($$
Product of all possible normal products $) \times ($ All possible contractions $)$
(23)

This is readily proven by induction (the proof can be found in most field theory texts). So, in the expansion of the Green's function, one just needs enough explicit creation and annihilation operators to give a non-vanishing matrix element; everything else is taken care of by the contractions.

5 Connection to the LSZ formula

The procedure above gives a diagrammatic representation of the S matrix. It is conceptually somewhat simpler than the LSZ discussion. But it relies on the identification of the initial and final states with their leading order expansions. We can refine this by thinking about the structure of the perturbation expansion. The LSZ formula systematizes this.

LSZ has other virtues. Most important, it is *not* a statement based on perturbation theory. It applies to *any* operator with matrix elements between the ground state and the single particle state of interest. So it can be used, for example, in strongly coupled theories like QCD.

The basic idea is that on shell Green's functions have poles; the coefficients of these poles, up to a constant, is the S matrix. Here we show that this is the case. We will be somewhat schematic; you are invited to fill in the details and make all of the steps rigourous. First, we review the idea of in and out states; this is already a notion which appears in quantum mechanical discussions of scattering (though often not in your first quantum course). Define the operator:

$$S = U(\infty, -\infty) \tag{24}$$

(U is the full time development operator). Then

$$\langle k_1, k_2, \dots k_n | S | p_1, \dots p_n \rangle$$

$$= \langle k_1, k_2, \dots k_n | e^{-iH(\infty - 0)} e^{-iH(0 - (-\infty))} | p_1, \dots p_n \rangle$$

$$\equiv _{out} \langle k_1, \dots k_n | p_1 \dots p_n \rangle_{in}.$$

$$(25)$$

For LSZ, we want to connect Green's functions, $\langle \Omega | \phi(x_1) \dots \phi(x_n) | \Omega \rangle$, Fourier transformed, to this object. For example, Fourier transforming in $x_1 \equiv x$, we want to study:

$$T \int d^4x e^{-ip \cdot x} \langle \Omega | \phi(x) \dots \phi(x_n) | \Omega \rangle.$$
(26)

Poles can only arise as one approaches infinity in the integrand. So take $x_0 \to -\infty$, $\vec{x} \to \infty$. Then the time ordering is easy; $\phi(x)$ stands to the right, and we can introduce a complete set of states:

$$\sum_{\lambda} \int \frac{d^3q}{(2\pi^3)2\omega(q)} \int d^4x e^{-ip \cdot x} \langle \Omega | \phi(x_2) \dots \phi(x_n) | \lambda_q \rangle \langle \lambda_q | \phi(x) | \Omega \rangle.$$
⁽²⁷⁾

Here the sum indicates labels of states other than the momentum. We can study the matrix element

$$\langle \lambda_q | \phi(x) | \Omega \rangle = \langle \lambda_q | e^{i \vec{P} \cdot \vec{x}} e^{-i P_0 x^0} e^{-i \vec{P} \cdot \vec{x}} e^{i P_0 x^0} \phi(x) e^{i \vec{P} \cdot \vec{x}} e^{-i P_0 x^0} e^{-i \vec{P} \cdot \vec{x}} e^{i P_0 x^0} \vec{\Omega} \rangle$$

$$= \langle \lambda_q | \phi(0) | \Omega \rangle e^{i q \cdot x_1}.$$

$$(28)$$

Now the integral over \vec{p} gives a δ function, $2\pi^3\delta(\vec{p}-\vec{q})$. The time integral diverges as $p_0 \rightarrow q_0$. Including a suitable $i\epsilon$ in the exponent to render the integral convergent (more precisely, one can think of this as adding a small imaginary part to p_0 ; the *S* matrix turns out to be analytic in momenta), one can do the p_0 integral. Combining the important factors:

$$\frac{1}{2\omega(p)}\frac{1}{p_0 - E(q) + i\epsilon} = -\frac{1}{p^2 + m^2 - i\epsilon}$$
(29)

implementing the delta function.

So far, this is quite similar to the manipulations used to derive the Kallen-Lehman representation. Now one repeats this process for the other fields. Here we have to be a bit more careful about what we take as the complete set of states. We start with asymptotic states which are well separated in space (wave packets) in the far past (or far future). Then most of the integral comes from the region where time is large and negative (or positive) and the states are still separated. The effect of the time evolution operator $(e^{iP^0x^0})$ is to yield the in and out states, with a phase like that above. Repeating iteratively, we obtain the full LSZ expression. The inputs are unitarity, and the assumption of a gap in the spectrum.