S-matrix and its connection to T-matrix.

Let us start with the evolution matrix in the interaction representation. It obeys the equation:

\[
\frac{dU(t, t_0)}{dt} = \frac{i}{\hbar} \tilde{V}(t) U(t, t_0)
\]

and the initial condition \( U(t_0, t_0) = I \). Here \( \tilde{V}(t) = e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar} \) is the interaction Hamiltonian in the interaction representation. For the scattering problem the interaction will be switched on adiabatically as \( V(t) = V e^{\gamma t} \), where \( \delta \) is very small positive value which will be put zero in the end. Then \( V(t) \) turns into zero at \( t \to -\infty \) and the Hamiltonian turns into that for free particle. The resulting transitions from initial state of the free Hamiltonian \( H_0 \) will be considered at \( t \to +\infty \), but in such a way that \( \gamma t \) remains much less than 1. In this limit the interaction Hamiltonian \( V(t) \) remains time independent at positive time. We will take \( t_0 = -\infty \). Integrating eq. (1) from \( -\infty \) till \( t \), we arrive at an integral equation (\( U(t) \equiv U(t, -\infty) \)):

\[
U(t) = I + \frac{1}{i\hbar} \int_{-\infty}^{t} \tilde{V}(t') U(t') dt'
\]

For matrix elements \( \langle n | U(t) | m \rangle = U_{nm}(t) \) one finds a system of linear integral equations:

\[
U_{nm}(t) = \delta_{n,m} + \frac{1}{i\hbar} \sum_k V_{nk} \int_{-\infty}^{t} e^{(i\omega_{nk} + \gamma)t'} U_{km}(t') dt',
\]

where \( \omega_{nm} = E_n - E_m \) are the transition frequencies of the Hamiltonian \( H_0 \). We look for a solution at time satisfying the condition \( \gamma |t| \ll 1 \) in the form:

\[
U_{nm}(t) = \delta_{n,m} - \frac{\Theta_{nm} e^{i\omega_{nm} t}}{\hbar (\omega_{nm} - i\gamma)}
\]

where the matrix \( \Theta_{nm} \) does not depend on time. Plugging eq. (4) into (3), we find a closed system of linear equations for the matrix elements \( T_{nm} \):

\[
\Theta_{nm} = V_{nm} - \sum_k \frac{V_{nk}}{\hbar (\omega_{km} - i\gamma)} \Theta_{km}
\]

It can be written in the operator form in a following way. Let us introduce an operator \( T(E) \) depending on the energy variable \( E \) and obeying equation:

\[
T = V + V (E - H_0 - i\gamma)^{-1} T
\]

Then the matrix \( T(E)_{nm} \) coincides with \( \Theta_{nm} \) at \( E = E_m \). To check this statement write eq. (6) in terms of matrix elements and put \( E = E_m \). You can see that the resulting system is the same as (5). Thus the relation between \( T \) and
\( \Theta \) operators can be formulated as \( \Theta = TP(E) \), where \( P(E) \) is the projection operator to the subspace of states with the energy \( E \). On the other hand, eq. (6) is identical with Lippmann-Schwinger equation. Therefore, the matrix \( T \) is identical with the Lippmann-Schwinger transition matrix.

The scattering matrix \( S \) is defined as \( S = U(+\infty,-\infty) = U(\infty) \). More accurately we have in mind the following limit: \( S = \lim_{t \rightarrow \infty, \delta \rightarrow 0, t \delta \rightarrow 0} U(t,-\infty) \). According to eq. (4), we need to find the limit:

\[
\lim_{t \rightarrow \infty, \gamma \rightarrow 0} e^{i\omega t} \omega - i\gamma
\]

We will show that it is equal to \( 2\pi i\delta(\omega) \). It is clear that the exponent \( e^{i\omega t} \) strongly oscillating as function of \( \omega \) at large \( t \) effectively cut the integration with any smooth function by the range \( \Delta \omega \sim 1/t \), whereas a typical denominator has the absolute value \( \sim 1/t \). Thus, it is delta-function with precision of a numerical factor. For finding of the numerical factor, we integrate the function under the sign of limit in eq. (7) by \( \omega \) from \(-\infty \) to \(+\infty \). Let us append it with the integral along infinite half-circle in the upper complex half-plane of \( \omega \). Since the exponent decreases at large positive \( 3\omega \), the integral over half-circle is zero. The contour encircles the pole at \( \omega = i\gamma \). The contribution of this pole is \( 2\pi i \). Thus, from eq. (4) we conclude that:

\[
S_{nm} = \delta_{nm} - 2\pi i\delta(E_n - E_m) \Theta_{nm}
\]

and taking in account the connection between operators \( \Theta \) and \( T \):

\[
S(E) = I - 2\pi i\delta(E - H_0) T(E) P(E)
\]

The operator \( S(E) \) conserves energy, i.e. its matrix elements are not zero only if the energies of both states are equal. Therefore it can be multiplied by projection operator \( P(E) \) left or right without changing the result. The operator \( S \) is unitary as a limit of unitary operator. Therefore it obeys the standard unitarity relation: \( SS^\dagger = I \). Employing eq. (9), one finds the unitarity condition in terms of the operator \( T \):

\[
iP(E) (T - T^\dagger) P(E) = -2\pi P(E) T\delta(E - H_0) T^\dagger P(E)
\]

Let us write this very general relation specifically for a particle scattered by potential. The states of the free Hamiltonian \( H_0 \) are labeled by the momentum \( p \). At a fixed value of \( E \) the momentum has modulus \( p = \sqrt{2mE} \), but its direction determined by a unit vector \( n \) remains arbitrary. Thus, all matrix elements \( \langle p | P(E) T P(E) | p' \rangle \) are functions of two unit vectors, which we denote \( T(n,n') \). In momentum representation equation (10) takes form:

\[
i[T(n,n') - T^*(n',n)] = -2\pi \int d^3p'' T(n,n'') \delta \left(E - \frac{P''^2}{2m}\right) T^*(n',n'')
\]

Representing the element of volume in the momentum space as \( d^3p'' = p''^2 dp'' d\Omega'' \) and performing integration over modulus \( p'' \), one finds:

\[
i[T(n,n') - T^*(n',n)] = -2\pi mp \int d\Omega'' T(n,n'') T^*(n',n'')
\]
Employing the relation between the scattering amplitude and transition matrix found earlier $f(n, \mathbf{n}') = -4\pi^2 m \hbar T(n, \mathbf{n}')$, the latter equation can be rewritten as equation for $f(n, \mathbf{n}')$:

$$i [f(n, \mathbf{n}') - f^*(\mathbf{n}', n)] = -\frac{k}{2\pi} \int d\Omega'' f(n, \mathbf{n}'') f^*(\mathbf{n}', \mathbf{n}'') \quad (13)$$

In particular the diagonal matrix element of this equation is the optic theorem:

$$\Im f(n, \mathbf{n}) = \frac{k}{4\pi} \sigma \quad (14)$$