The transition operator is an operator which contains all the information necessary to construct the exact scattering amplitude in a scattering problem. It is particularly convenient for exploring the effects of symmetries on the cross section. These notes concern the transition operator and some related issues concerning Green’s operators.

We begin with the Lippmann-Schwinger equation (29.73), which we write in the form

$$|\phi_k\rangle = [1 - G_{0+}(E)V]|\psi_k\rangle.$$  \hspace{1cm} (30.1)

This form shows quite clearly that the Lippmann-Schwinger equation is not a solution for the exact scattered wave field $|\psi_k\rangle$, although if $|\psi_k\rangle$ were known, the Lippmann-Schwinger equation could be used to determine the incident plane wave $|\phi_k\rangle$ associated with it. This, of course, would not be very useful.

On the other hand, if we could find the inverse of the operator $1 - G_{0+}(E)V$, then we could solve for $|\psi_k\rangle$ in terms of $|\phi_k\rangle$. One approach to finding this inverse is simply to treat $G_{0+}(E)V$ as small, and expand in a Taylor series. This gives

$$[1 - G_{0+}(E)V]^{-1} = \sum_{n=0}^{\infty} [G_{0+}(E)V]^n,$$  \hspace{1cm} (30.2)

which, when applied to $|\phi_k\rangle$, simply reproduces the Born series which we obtained earlier by iterating the Lippmann-Schwinger equation. The trouble with the Born series, however, is that the integrals involved in the higher order terms may not be easy to do, and in any case the series may not converge. Certainly the Born series is not useful when the potential causes a significant distortion in the incident wave in the region where $V \neq 0$.

It turns out that the desired inverse can be expressed in terms of the exact Green’s operator for the system. Recall that we are writing $H = H_0 + V$, where $H_0 = p^2/2m$ is the unperturbed, free particle Hamiltonian, and $H_1 = V$ is the perturbation. The unperturbed and exact Green’s operators are defined by

$$G_0(z) = \frac{1}{z - H_0}, \quad G(z) = \frac{1}{z - H},$$  \hspace{1cm} (30.3)

where to avoid singularities we have set $z = E + i\epsilon$ to push the energy into the upper half complex energy plane. The Green’s operators $G_{0+}(E)$ and $G_+(E)$ are then obtained by
taking the limit $\epsilon \to 0$, which exists as long as we avoid the discrete eigenvalues of either $H_0$ or $H$ (of course, the free particle Hamiltonian $H_0$ has no discrete eigenvalues).

Actually, the specific forms of $H_0$ and $H_1$ are not important for much of the following analysis, so our results will not be limited to scattering problems of the specific form we have chosen (nonrelativistic potential scattering of spinless particles). For example, most of the results presented in these Notes can be applied to problems involving the emission and absorption of photons, or to relativistic and field theoretic problems of various kinds.

We will now express the inverse of of $1 - G_0(z)V$ in terms of the exact Green’s operator $G(z)$. This is fairly easy; we simply write

$$1 - G_0(z)V = 1 - \frac{1}{z - H_0}V = \frac{1}{z - H_0}(z - H_0 - V) = \frac{1}{z - H_0}(z - H),$$

so that

$$[1 - G_0(z)V]^{-1} = \frac{1}{z - H}(z - H_0) = \frac{1}{z - H}(z - H_0 - V + V)$$

$$= G(z)(z - H + V) = 1 + G(z)V.$$  \hspace{1cm} (30.5)

We can summarize this identity by writing,

$$[1 - G_0(z)V][1 + G(z)V] = [1 + G(z)V][1 - G_0(z)V] = 1.$$ \hspace{1cm} (30.6)

Now the solution of the Lippmann-Schwinger equation can be written in the form,

$$|\psi_k\rangle = [1 + G_+(E)V]|\phi_k\rangle,$$ \hspace{1cm} (30.7)

where we have used Eq. (30.6) and taken $\epsilon \to 0$. We see that knowledge of the exact Green’s operator for the system is equivalent to the knowledge of the exact scattering solution (we need only carry out a single integral to obtain the scattered wave function). As pointed out in Notes 29, knowledge of the exact Green’s operator $G(z)$ is also equivalent to the knowledge of the bound state energy levels and eigenfunctions. These facts make the Green’s operator an interesting object, but they also mean that in practice we seldom know what the exact Green’s operator is, because we seldom have such a complete solution of a quantum mechanical problem. Nevertheless, the Green’s operator is important for many purposes, including the construction of approximation methods.

The result (30.7) can be understood from another standpoint. Imagine a world in which we could easily solve the exact Schrödinger equation,

$$(H - E)|\psi\rangle = 0,$$ \hspace{1cm} (30.8)
including the exact scattering problem in the continuous spectrum, but we could not solve
the unperturbed problem,
\[(H_0 - E)|\phi\rangle = 0, \quad (30.9)\]
whose solutions are of course plane waves. How could we use the knowledge of the solutions
of Eq. (30.8) to find those of Eq. (30.9)? One way would be to proceed exactly as we did
in Notes 29, by rewriting Eq. (30.9) in the form
\[(H_0 + V - E)|\phi\rangle = (H - E)|\phi\rangle = V|\phi\rangle, \quad (30.10)\]
whereupon the right hand side appears as a source or driving term for the otherwise ho-
mogeneous equation (30.8). Then the general solution of Eq. (30.10) could be written as
a solution of the homogeneous equation (30.8) plus an integral of the Green’s function for
Eq. (30.8) over the driving term. Using the property (29.28) of the Green’s operator, we
can write the result in operator language,
\[|\phi\rangle = |\psi\rangle - G_+(E)V|\phi\rangle. \quad (30.11)\]
This is the same as Eq. (30.7).

We see that there is a kind of reciprocity between the exact and plane wave problems,
and that correct formulas usually result if we take any correct formula and swap the symbols,
\[H_0 \leftrightarrow H, \ G_0 \leftrightarrow G, \ V \leftrightarrow -V, \ \text{and} \ |\phi\rangle \leftrightarrow |\psi\rangle.\] An example where this works is the Lippmann-
Schwinger equation itself, or Eq. (30.6).

There is another useful relation between the exact and unperturbed Green’s operators,
which is closely related to Eq. (30.6). This is
\[G(z) = G_0(z) + G_0(z)VG(z) = G_0(z) + G(z)VG_0(z). \quad (30.12)\]
This identity is presented in two forms, differing by the order of the operators in the second
term. We can easily prove the first form. We simply write
\[G_0(z) + G_0(z)VG(z) = G_0(z)[1 + VG(z)] = \frac{1}{z - H_0}\left[1 + V\frac{1}{z - H}\right]
= \frac{1}{z - H_0}(z - H + V)\frac{1}{z - H} = G_0(z)(z - H_0)G(z) = G(z). \quad (30.13)\]
The second form is proved similarly.

The first form can be regarded as a kind of Lippmann-Schwinger equation for the exact
Green’s operator, for if it is written out in terms of the corresponding Green’s function, it
becomes
\[G(r, r', z) = G_0(r, r', z) + \int d^3r'' G_0(r, r'', z)V(r'')G(r'', r', z), \quad (30.14)\]
which should be compared to Eq. (29.9). In this equation we may think of the unperturbed Green’s function $G_0$ as known, and the exact Green’s function $G$ as unknown (the usual situation). According to this equation, the $r$ dependence of the exact Green’s function $G$ satisfies the usual Lippmann-Schwinger equation [see Eq. (29.9)]. The second form of the identity (30.12) is also a kind of Lippmann-Schwinger equation, but now when we put it into wave function language, it involves the $r'$ dependence of $G$:

$$G(r, r', z) = G_0(r, r', z) + \int d^3r'' G(r, r'', z) V(r'') G_0(r'', r', z).$$

(30.15)

Obviously, finding the exact Green’s operator is equivalent to, and just as hard, as solving the Lippmann-Schwinger equation for the exact scattering solutions $|\psi_k\rangle$.

The relation (30.12) can be solved for the exact Green’s operator by expanding in a kind of Born series:

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots = \sum_{n=0}^{\infty} (G_0 V)^n G_0 = G_0 \sum_{n=0}^{\infty} (V G_0)^n,$$

(30.16)

where $G = G(z)$ and $G_0 = G_0(z)$.

Let us return to Eq. (29.72) for the scattering amplitude $f(k, k')$. (This notation is slightly misleading. The scattering amplitude $f$ does not depend on the two vectors $k$ and $k'$ independently, because their magnitudes are equal, $k = k'$.) We use Eq. (30.7) in Eq. (29.72) to write

$$f(k, k') = -\frac{4\pi^2 m}{\hbar^2} \langle \phi_{k'} | T(E) | \phi_{k} \rangle,$$

(30.17)

where we define

$$T(E) = V + VG_+ (E) V.$$

(30.18)

The operator $T(E)$ is the transition operator. Equation (30.17) is a somewhat more symmetrical representation of the scattering amplitude than Eq. (29.72), because we have plane wave states on both sides of the matrix element. The transition operator incorporates all the complexities of the scattering process, and Eq. (30.17) is exact. Notice that if $T(E)$ is replaced by the potential $V$, we obtain the approximate scattering amplitude of the first Born approximation, or of first order time-dependent perturbation theory. The transition operator is not Hermitian, but rather satisfies

$$T(E)\dagger = V + VG_- (E) V,$$

(30.19)

where we use the fact that $[G_+(E)]\dagger = G_-(E)$.

The transition operator, or $T$-operator for short, is useful for exploring the effects of symmetry on the scattering amplitude. Let us begin with parity. We denote the parity
operator by \( \pi \), so that \( \pi^\dagger \pi = 1 \). The action of parity on plane wave states is given by \( \pi |k\rangle = |-k\rangle \). (Here the plane wave \( |k\rangle \) is the same as \( |\phi_k\rangle \).) Suppose that the Hamiltonian commutes with parity, so that \([\pi, H] = 0\) and \([\pi, V] = 0\). Then \( \pi \) commutes with any function of \( H \), so that

\[
[\pi, G(z)] = \left[ \pi, \frac{1}{z - H} \right] = 0.
\]

From this and Eq. (30.18) it follow that \([\pi, T(E)] = 0\). Then we have

\[
(k'|T(E)|k) = (k'|\pi^\dagger T(E)\pi^\dagger |k\rangle = (-k'|T(E)|-k),
\]

or,

\[
f(k', k) = f(-k', -k).
\]

This is illustrated as case (a) in Fig. 30.1.

![Fig. 30.1. Effects of various symmetries on the scattering amplitude: (a), parity; (b), time-reversal; (c), parity and time-reversal.](image)

Next let us consider the effects of time-reversal invariance. We denote the time-reversal operator by \( \Theta \); it is antiunitary, and satisfies \( \Theta^\dagger \Theta = 1 \). The action of time-reversal on the (spinless) plane wave states is given by \( \Theta |k\rangle = |-k\rangle \), since the wave function \( e^{i\mathbf{k} \cdot \mathbf{r}} \) is transformed into its complex conjugate \( e^{-i\mathbf{k} \cdot \mathbf{r}} \) [see Eq. (17.45)]. Suppose that \( \Theta \) commutes with the Hamiltonian \( H \), and therefore with \( V \), \([\Theta, H] = [\Theta, V] = 0\). This does not mean that \( \Theta \) commutes with \( G_+(E) \), for we have

\[
\Theta G_+(E) \Theta^\dagger = \Theta \left( \lim_{\epsilon \to 0} \frac{1}{E + i\epsilon - H} \right) \Theta^\dagger = \lim_{\epsilon \to 0} \frac{1}{E - i\epsilon - H} = G_-(E),
\]

(30.23)
since the antiunitary $\Theta$ turns $E + i\epsilon$ into $E - i\epsilon$. (More pictorially, we can say that reversing the direction of time turns the outgoing Green’s operator into the incoming Green’s operator.) Now Eqs. (30.18), (30.19), and (30.23) imply

$$\Theta T(E)\Theta^\dagger = T(E)^\dagger.$$  \hfill (30.24)

Now let us examine the effect of time-reversal invariance on the matrix elements of the $T$-operator. We have

$$\langle k' | T(E) | k \rangle = \langle k' | (\Theta^\dagger T(E)\Theta^\dagger \Theta | k) \rangle = \langle k' | (\Theta^\dagger T(E)^\dagger | -k) \rangle$$

$$= \langle -k' | T(E)^\dagger | -k \rangle^* = \langle -k | T(E) | -k' \rangle,$$  \hfill (30.25)

where the parentheses are used to indicate that the time-reversal operators act to the right, and where in the third equality we have reversed the direction in which $\Theta^\dagger$ is acting, and used Eq. (17.21). Thus, time reversal invariance implies that the scattering amplitude satisfies

$$f(k, k') = f(-k', -k).$$  \hfill (30.26)

This property is called microreversibility, and it is illustrated in case (b) in Fig. 30.1.

Finally, if both parity and time-reversal are symmetries of the Hamiltonian, then we have

$$f(k, k') = f(k', k).$$  \hfill (30.27)

This property is called detailed balance, and it is illustrated in case (c) in Fig. 30.1.

As a final topic, let us derive the orthonormality conditions for the exact scattering states $|\psi_k\rangle$. These conditions are not easy to derive directly from the Schrödinger equation or from the integral equation (29.9), but they can be easily obtained with the help of our various identities involving Green’s operators. We begin by using Eq. (30.7) to transform the scalar product of two exact scattering states,

$$\langle \psi_{k'} | \psi_k \rangle = \langle \psi_{k'} | \phi_k \rangle + \langle \psi_{k'} | G_+(E)V | \phi_k \rangle.$$  \hfill (30.28)

The second term of this equation can be written,

$$\langle \psi_{k'} | G_+(E)V | \phi_k \rangle = \lim_{\epsilon \to 0} \langle \psi_{k'} | \frac{1}{E + i\epsilon - H} V | \phi_k \rangle = \lim_{\epsilon \to 0} \frac{1}{E + i\epsilon - E'} \langle \psi_{k'} | V | \phi_k \rangle.$$  \hfill (30.29)

Here $E = \hbar^2 k^2 / 2m$ and $E' = \hbar^2 k'^2 / 2m$. But the first term on the right in Eq. (30.28) can be transformed with the help of the Hermitian conjugate the Lippmann-Schwinger equation (29.73),

$$\langle \psi_{k'} | \phi_k \rangle = \langle \phi_{k'} | \phi_k \rangle + \langle \psi_{k'} | VG_0-(E') | \phi_k \rangle = \delta(k - k') + \lim_{\epsilon \to 0} \langle \psi_{k'} | V \frac{1}{E' - i\epsilon - H_0} | \phi_k \rangle$$

$$= \delta(k - k') + \lim_{\epsilon \to 0} \frac{1}{E' - i\epsilon - E} \langle \psi_{k'} | V | \phi_k \rangle.$$  \hfill (30.30)
When we combine these equations, we obtain

$$
\langle \psi_{k'} | \psi_k \rangle = \delta(k - k'),
$$

(30.31)
a simple result.

Although the exact scattering states $|\psi_k\rangle$ are orthonormal, they are not complete in general, because of bound states. All bound states of the Hamiltonian $H$ are orthogonal to all scattering states,

$$
\langle n\alpha | \psi_k \rangle = 0,
$$

(30.32)
as is easily proved with the help of the integral equation (29.75). The completeness relation relation is

$$
\sum_{n\alpha} |n\alpha\rangle \langle n\alpha| + \int d^3k |\psi_k\rangle \langle \psi_k| = 1.
$$

(30.33)
This can be proved by a contour integration which inverts the definition of the Green’s operators. We will not go into details here.