

Scattering Theory

In quantum mechanics the basic observable is the probability

$$P = |\langle \psi^+(t) | \psi^-(t) \rangle|^2, \quad (1)$$

for a transition from an initial state, $|\psi^-(t)\rangle$, to a final state, $|\psi^+(t)\rangle$. Since time evolution is unitary this probability is independent of time and can be evaluated at any time t :

$$\begin{aligned} P(t) &= |\langle \psi^+(t) | \psi^-(t) \rangle|^2 = |\langle \psi^+(0) | e^{iHt/\hbar} e^{-iHt/\hbar} \psi^-(0) \rangle|^2 = \\ &= |\langle \psi^+(0) | \psi^-(0) \rangle|^2 = P(0). \end{aligned} \quad (2)$$

For a scattering experiment $|\psi^-(t)\rangle$ represents the state of the beam and target at time t . It is a solution of the Schrödinger equation that looks like a free beam particle heading towards a free target particle at a time $t = -T$, when the beam and target are initially prepared (long before the collision). Similarly $|\psi^+(t)\rangle$ is a solution of the Schrödinger equation that represents the state selected by the detectors. At the time $t = T$, long after the collision, this state looks like two free particles heading towards specific elements of the detector, for example towards a particular pair of photo-multiplier tubes. The probability (1) is the probability that the initial state will be measured in the final state.

The scattering probability must be evaluated at a common time for both the initial and final states. The problem is that there is no single time where both the initial and final state look like free particles.

The initial conditions for the two solutions of the Schrödinger equation are most naturally formulated at the times $-T$ and T when the initial and final states behave like states of free particles:

$$i\hbar \frac{d}{dt} |\Psi^\pm(t)\rangle = H |\Psi^\pm(t)\rangle, \quad |\Psi^\pm(\pm T)\rangle = |\Psi_0^\pm(\pm T)\rangle \quad (3)$$

where

$$|\Psi_0^\pm(\pm T)\rangle \quad (4)$$

are the corresponding non-interacting solutions at $t = -T$ and $t = T$. The states (4) are solutions of the free-particle Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi_0^\pm(t)\rangle = H_0 |\Psi_0^\pm(t)\rangle. \quad (5)$$

The solutions $|\Psi^\pm(t)\rangle$ and $|\Psi_0^\pm(t)\rangle$, of equations (3) and (5) can be expressed in terms of the unitary time evolution operators $U(t)$ and $U_0(t)$ and the initial conditions:

$$|\Psi^\pm(t)\rangle = U(t \mp T) |\Psi^\pm(\pm T)\rangle \quad U(t) = e^{-iHt/\hbar} \quad (6)$$

$$|\Psi_0^\pm(t)\rangle = U_0(t \mp T) |\Psi^\pm(T)\rangle \quad U_0(t) = e^{-iH_0 t/\hbar}. \quad (7)$$

The initial free particle wave packets can be taken as minimal uncertainty wave packets with momentum uncertainty $\Delta \mathbf{p}_1$ and $\Delta \mathbf{p}_2$ and specified mean single-particle momenta, \mathbf{p}_{10} and \mathbf{p}_{20} . The minimal uncertainty states have the form

$$\langle \mathbf{p}_1, \mathbf{p}_2 | \Psi_0^\pm(t) \rangle = \frac{1}{(2\pi)^{3/4}} \frac{1}{(\Delta \mathbf{p}_1)^{3/2}} e^{-\frac{(\mathbf{p}_1 - \mathbf{p}_{10})^2}{(2\Delta \mathbf{p}_1)^2}} \frac{1}{(2\pi)^{3/4}} \frac{1}{(\Delta \mathbf{p}_2)^{3/2}} e^{-\frac{(\mathbf{p}_2 - \mathbf{p}_{20})^2}{(2\Delta \mathbf{p}_2)^2}} e^{-i(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2})t/\hbar}. \quad (8)$$

In an actual experiment there is no precise control over the structure of the initial or final wave packets. For example the particle might be detected in the photo-multiplier tubes in a state orthogonal to $|\Psi^+(T)\rangle$. What is really in an experiment is counts in a detector like a photo-multiplier tube. It is also awkward to determine the precise value of $\pm T$. For these reason scattering theory is formulated in a manner that removes the sensitivity to the choice of wave packet or T provided the wave packets are sufficiently narrow in momentum and the times T are sufficiently large. How this is achieved is discussed in what follows.

To remove the dependence on the choice of T note that once the particles are beyond the range of the interaction, H acts like the free Hamiltonian H_0 and the unitary time-evolution operator $U(t)$ can be replaced by the free time-evolution operator $U(t) = e^{-iHt/\hbar} \rightarrow U_0(t) = e^{-iH_0t/\hbar}$. This means that if

$$|\Psi^\pm(\pm T)\rangle = |\Psi_0^\pm(\pm T)\rangle \quad (9)$$

at times $t = \pm T$ then at times $t = \pm(T + \Delta t)$ the states are still approximately equal

$$|\Psi^\pm(\pm(T + \Delta T))\rangle = U(\pm \Delta T) |\Psi^\pm(\pm T)\rangle \approx U_0(\pm \Delta T) |\Psi^\pm(\pm T)\rangle = U_0(\pm \Delta T) |\Psi_0^\pm(\pm T)\rangle = |\Psi_0^\pm(\pm(T + \Delta T))\rangle, \quad (10)$$

which shows that the initial conditions at $\pm T$ are approximately equivalent to initial conditions at $\pm(T + \Delta T)$ for any positive ΔT . The T dependence can be eliminated by taking the limit $T \rightarrow \infty$, which does not change the initial condition for short range V . This leads to the **scattering asymptotic conditions**:

$$\begin{aligned} 0 &= \lim_{t \rightarrow \pm\infty} \| |\Psi^\pm(t)\rangle - |\Psi_0^\pm(t)\rangle \| = \\ &= \lim_{t \rightarrow \pm\infty} \| e^{-iH\frac{t}{\hbar}} |\Psi^\pm(0)\rangle - e^{-iH_0\frac{t}{\hbar}} |\Psi_0^\pm(0)\rangle \| = \\ &= \lim_{t \rightarrow \pm\infty} \| |\Psi^\pm(0)\rangle - e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}} |\Psi_0^\pm(0)\rangle \| \end{aligned} \quad (11)$$

where the unitarity of the time evolution operator, $\|e^{iH\frac{t}{\hbar}}|\Psi\rangle\| = \|\Psi\rangle\|$ was used in the last line of (11). This condition can be written as

$$|\Psi^\pm(0)\rangle = \lim_{t \rightarrow \pm\infty} e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}} |\Psi_0^\pm(0)\rangle = \Omega_\pm |\Phi_0^\pm(0)\rangle. \quad (12)$$

The operators,

$$\Omega_\pm := \lim_{t \rightarrow \pm\infty} e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}}, \quad (13)$$

are called **Møller wave operators**. The limit is a strong limit. This means that it is only defined when the operators are applied to wave packets, as they are in (11). The existence of this limit can be proven for a large class of short-ranged interactions (a notable exception is the Coulomb interaction - this will be discussed separately.) Sufficient conditions for the existence of the wave operators follow by writing the limit (13) as an integral of a derivative

$$\begin{aligned}\Omega_{\pm} &:= I + \int_0^{\pm\infty} \frac{d}{dt} e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}} dt = \\ &I + \frac{i}{\hbar} \int_0^{\pm\infty} e^{iH\frac{t}{\hbar}} V e^{-iH_0\frac{t}{\hbar}} dt.\end{aligned}$$

Convergence follows provided

$$\left\| \int_0^{\pm\infty} e^{iH\frac{t}{\hbar}} V e^{-iH_0\frac{t}{\hbar}} dt |\psi\rangle \right\| < \infty.$$

A sufficient condition for this to be finite is

$$\int_0^{\infty} \|V e^{\mp iH_0\frac{t}{\hbar}} |\psi\rangle\| dt < \infty. \quad (14)$$

Condition (14) is called the **Cook condition**. Whether this is satisfied depends on the choice of potential. It holds for most potentials that fall off faster than the Coulomb potential at ∞ . In what follows the Møller wave operators are assumed to exist.

The Møller wave operators satisfy the **intertwining relations**

$$H\Omega_{\pm} = \Omega_{\pm}H_0. \quad (15)$$

To prove (15) note that

$$e^{iH\frac{s}{\hbar}}\Omega_{\pm} = \lim_{(t+s)\rightarrow\pm\infty} e^{iH\frac{(t+s)}{\hbar}} e^{-iH_0\frac{(t+s)}{\hbar}} e^{iH_0\frac{s}{\hbar}} = \Omega_{\pm} e^{iH_0\frac{s}{\hbar}}. \quad (16)$$

Differentiation with respect to s , setting s to zero gives (15). This condition ensures that energy is conserved in the scattering experiment; i.e. that

$$H\Omega_{\pm}|E_0\rangle = \Omega_{\pm}H_0|E_0\rangle = E_0\Omega_{\pm}|E_0\rangle. \quad (17)$$

This must be true since the interacting states become non-interacting when the particle are beyond the range of the interaction. Equation (17) shows that Ω_{\pm} maps eigenstates of H_0 with energy E_0 to eigenstates of H with the same energy.

It also follows that

$$\begin{aligned}|\Psi^{\pm}(t)\rangle &= U(t)|\Psi^{\pm}(0)\rangle = \\ U(t)\Omega_{\pm}|\Psi_0^{\pm}(0)\rangle &= \Omega_{\pm}U_0(t)|\Psi_0^{\pm}(0)\rangle = \Omega_{\pm}|\Psi_0^{\pm}(t)\rangle.\end{aligned} \quad (18)$$

The scattering probability can be expressed directly in terms of the asymptotic free-particle wave packets using the Møller operators:

$$P = |\langle \Psi_0^+(t) | \Omega_+^\dagger \Omega_- | \Psi_0^-(t) \rangle|^2 \quad (19)$$

which is independent of t by (18).

The **scattering operator** S is defined by

$$S := \Omega_+^\dagger \Omega_-. \quad (20)$$

The scattering probability can be expressed in terms of the free-particle asymptotic states and S as

$$P = |\langle \Psi_0^+(t) | S | \Psi_0^-(t) \rangle|^2. \quad (21)$$

The advantage of expressing the probability in terms of the free-particle states is that they have a simple form that is determined by the quantities that can be controlled in an experiment like the beam and target momenta and well as the position and resolution of the detectors. These quantities are independent of the interaction. The physics associated with the interaction is contained in the operator S .

There are a number of ways to calculate the scattering operator S . All of them involve closely related quantities.

Structure of the scattering operator

Scattering probability amplitude can be expressed in term of free-particle matrix elements of the scattering operator

$$\begin{aligned} \langle \Psi_0^+ | S | \Psi_0^- \rangle = \\ \int \langle \Psi_0^+ | \mathbf{p}_1, \mathbf{p}_2 \rangle d\mathbf{p}_1 d\mathbf{p}_2 \langle \mathbf{p}_1, \mathbf{p}_2 | S | \mathbf{p}'_1, \mathbf{p}'_2 \rangle d\mathbf{p}'_1 d\mathbf{p}'_2 \langle \mathbf{p}'_1, \mathbf{p}'_2 | \Psi_0^- \rangle. \end{aligned} \quad (22)$$

Since typical interactions are translationally invariant, for some purposes it is useful to change variables to the total momentum of the system,

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad (23)$$

which is conserved and the momentum of particle 1 in the two-body rest frame:

$$\mathbf{k} := \mathbf{p}_1 - \frac{m_1}{m_1 + m_2} \mathbf{P} = \frac{m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2}{m_1 + m_2}, \quad (24)$$

where \mathbf{P} is the total momentum of the two-body system, and \mathbf{k} is the momentum of particle 1 in the frame where $\mathbf{P} = 0$. This is just a Galilean boost by velocity $\mathbf{v} = -\mathbf{P}/(m_1 + m_2)$. We also have

$$-\mathbf{k} := \mathbf{p}_2 - \frac{m_1}{m_1 + m_2} \mathbf{P} = \frac{m_1 \mathbf{p}_2 - m_2 \mathbf{p}_1}{m_1 + m_2}. \quad (25)$$

The Jacobian of the variable change

$$(\mathbf{p}_1, \mathbf{p}_2) \rightarrow (\mathbf{P}, \mathbf{k}) \quad (26)$$

is 1.

In terms of the variables \mathbf{P} and \mathbf{k} the scattering probability amplitude can be expressed as

$$\int \langle \Psi_0^+ | \mathbf{k}, \mathbf{P} \rangle d\mathbf{k} d\mathbf{P} \langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle d\mathbf{k}' d\mathbf{P}' \langle \mathbf{k}', \mathbf{P}' | \Psi_0^- \rangle. \quad (27)$$

The kernel of the scattering operator in these variables has the form

$$\begin{aligned} \langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle &= \\ \lim_{t \rightarrow \infty} \langle \mathbf{k}, \mathbf{P} | e^{iH_0 t/\hbar} e^{-2iHt/\hbar} e^{iH_0 t/\hbar} | \mathbf{k}', \mathbf{P}' \rangle &= \\ \delta(\mathbf{P} - \mathbf{P}') \delta(\mathbf{k} - \mathbf{k}') + \int_0^\infty \frac{d}{dt} \langle \mathbf{k}, \mathbf{P} | e^{iH_0 t/\hbar} e^{-2iHt/\hbar} e^{iH_0 t/\hbar} | \mathbf{k}', \mathbf{P}' \rangle &= \\ \delta(\mathbf{P} - \mathbf{P}') \delta(\mathbf{k} - \mathbf{k}') - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k}, \mathbf{P} | e^{iH_0 t/\hbar} V e^{-2iHt/\hbar} e^{iH_0 t/\hbar} | \mathbf{k}', \mathbf{P}' \rangle - & \\ \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k}, \mathbf{P} | e^{iH_0 t/\hbar} e^{-2iHt/\hbar} V e^{iH_0 t/\hbar} | \mathbf{k}', \mathbf{P}' \rangle & \end{aligned} \quad (28)$$

where the chain rule was used to differentiate the product $(e^{iH_0 t/\hbar} e^{-iHt/\hbar}) \times (e^{-2iHt/\hbar} e^{iH_0 t/\hbar})$ in (28).

We define \mathbf{h} and h_0 (the rest energy operators) in terms of the free and interacting Hamiltonians by

$$H = \frac{\mathbf{P}^2}{2M} + h \quad h = \frac{\mathbf{k}^2}{2\mu} + V \quad (29)$$

$$H_0 = \frac{\mathbf{P}^2}{2M} + h_0 \quad h_0 = \frac{\mathbf{k}^2}{2\mu}. \quad (30)$$

If the interaction is translationally invariant, $[V, \mathbf{P}] = 0$, then

$$e^{iHt/\hbar} e^{-iH_0 t/\hbar} = e^{iht/\hbar} e^{-ih_0 t/\hbar}. \quad (31)$$

If the interaction is translationally invariant, i.e. $[H, \mathbf{P}] = [H_0, \mathbf{P}] = 0$, then a total momentum conserving delta function can be factored out and \mathbf{H} and H_0 can be replaced by h and h_0 . In what follows “hats” are used to indicate operators with the momentum conserving delta function removed

$$\langle \mathbf{P}, \mathbf{k} | O | \mathbf{P}', \mathbf{k}' \rangle =: \delta(\mathbf{P} - \mathbf{P}') \langle \mathbf{k} | \hat{O} | \mathbf{k}' \rangle. \quad (32)$$

Thus, assuming a translationally invariant interaction, equation (28) becomes

$$\langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle =$$

$$\delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{ih_0 t/\hbar} \hat{V} e^{-2iht/\hbar} e^{ih_0 t/\hbar} | \mathbf{k}' \rangle - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{ih_0 t/\hbar} e^{-2iht/\hbar} \hat{V} e^{ih_0 t/\hbar} | \mathbf{k}' \rangle \right). \quad (33)$$

Note that $|\mathbf{k}\rangle$ is an eigenstate of h_0 with eigenvalue $E(\mathbf{k}) = \frac{\mathbf{k}^2}{2\mu}$:

$$h_0 |\mathbf{k}\rangle = \frac{\mathbf{k}^2}{2\mu} |\mathbf{k}\rangle = E(\mathbf{k}) |\mathbf{k}\rangle. \quad (34)$$

The average relative kinetic energy is defined by

$$\bar{E} = \frac{1}{2} (E(\mathbf{k}) + E(\mathbf{k}')). \quad (35)$$

Using (34) and (35) in (33) gives

$$\begin{aligned} \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{ih_0 t/\hbar} \hat{V} e^{-2iht/\hbar} e^{ih_0 t/\hbar} | \mathbf{k}' \rangle - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{ih_0 t/\hbar} e^{-2iht/\hbar} \hat{V} e^{ih_0 t/\hbar} | \mathbf{k}' \rangle \right) = \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | \hat{V} e^{-2i(h-\bar{E})t/\hbar} | \mathbf{k}' \rangle - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{-2i(h-\bar{E})t/\hbar} \hat{V} | \mathbf{k}' \rangle \right). \end{aligned} \quad (36)$$

The time integrals only converge if the kernel is *first* integrated over the wave packets in (27). The important observation is that the order of performing the integrals matters in these expressions. When the integrals over \mathbf{k}, \mathbf{P} and \mathbf{k}' are performed *before* the time integrals, the resulting time-dependent integrand will vanish for large t . This can be seen by considering the example

$$\begin{aligned} \int f(\mathbf{k}) e^{\frac{-i\mathbf{k}^2 t}{2\mu\hbar}} d^3 \mathbf{k} = \int \hat{f}(k^2) e^{\frac{-ik^2 t}{2\mu\hbar}} k^2 dk = \\ \left(\frac{2\mu\hbar}{t} \right)^{3/2} \int \hat{f}\left(\frac{2\mu\hbar}{t} u^2\right) e^{-iu^2} u^2 du \end{aligned} \quad (37)$$

where

$$\hat{f}(k^2) := \int f(\mathbf{k}) d\hat{\mathbf{k}} \quad (38)$$

This falls off like $t^{-3/2}$ for large t . If an additional factor $e^{-\epsilon t}$ is inserted where ϵ small enough so $e^{-\epsilon t} \approx 1$ for all t where the integrand is non-zero, then this addition will not affect the value of the integral in the limit that $\epsilon \rightarrow 0$. This fall off, due to the spreading of the wave packet, is responsible for the convergence of the Cook condition, (14). When the factor $e^{-\epsilon t}$ is included the time and momentum integrals can be computed in any order. For computational

purposes it is useful to include the $e^{-\epsilon t}$ and perform the time integral first, with the understanding that $\lim_{\epsilon \rightarrow 0}$ be taken *after* integrating over the initial and final wave packets. It follows that (36) can be replaced by

$$\begin{aligned} \langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle = \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | \hat{V} e^{-2i(h - \bar{E} - i\epsilon)t/\hbar} | \mathbf{k}' \rangle - \right. \\ \left. \frac{i}{\hbar} \int_0^\infty \langle \mathbf{k} | e^{-2i(h - \bar{E} - i\epsilon)t/\hbar} \hat{V} | \mathbf{k}' \rangle \right) \end{aligned} \quad (39)$$

Doing the time integral gives

$$\begin{aligned} \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') + \frac{1}{2} \langle \mathbf{k} | \hat{V} \frac{1}{\bar{E} - h + i\epsilon} | \mathbf{k}' \rangle + \right. \\ \left. + \frac{1}{2} \langle \mathbf{k} | \frac{1}{\bar{E} - h + i\epsilon} \hat{V} | \mathbf{k}' \rangle \right) \end{aligned} \quad (40)$$

Some care is required to evaluate (40). The second resolvent identities

$$\frac{1}{z - A} - \frac{1}{z - B} = \frac{1}{z - A} (A - B) \frac{1}{z - B} = \frac{1}{z - B} (A - B) \frac{1}{z - A} \quad (41)$$

can be applied to h and h_0 with $z = \bar{E} + i\epsilon$:

$$\begin{aligned} \frac{1}{\bar{E} - h + i\epsilon} - \frac{1}{\bar{E} - h_0 + i\epsilon} = \\ \frac{1}{\bar{E} - h_0 + i\epsilon} V \frac{1}{\bar{E} - h + i\epsilon} = \frac{1}{\bar{E} - h + i\epsilon} V \frac{1}{\bar{E} - h_0 + i\epsilon}. \end{aligned} \quad (42)$$

Using (42) in (40) gives

$$\begin{aligned} \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') + \frac{1}{2} \langle \mathbf{k} | \hat{V} (1 + \frac{1}{\bar{E} - h + i\epsilon} \hat{V}) \frac{1}{\bar{E} - h_0 + i\epsilon} | \mathbf{k}' \rangle + \right. \\ \left. + \frac{1}{2} \langle \mathbf{k} | \frac{1}{\bar{E} - h_0 + i\epsilon} (1 + \hat{V} \frac{1}{\bar{E} - h + i\epsilon} \hat{V}) | \mathbf{k}' \rangle \right) = \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') + \frac{1}{2} \langle \mathbf{k} | (\hat{V} + \hat{V} \frac{1}{\bar{E} - h + i\epsilon} \hat{V}) | \mathbf{k}' \rangle \left(\frac{1}{\bar{E} - E(k') + i\epsilon} + \frac{1}{\bar{E} - E(k) + i\epsilon} \right) \right) \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') + \frac{1}{2} \langle \mathbf{k} | (\hat{V} + \hat{V} \frac{1}{\bar{E} - h + i\epsilon} \hat{V}) | \mathbf{k}' \rangle \left(\frac{1}{\bar{E} - E(k') + i\epsilon} + \frac{1}{\bar{E} - E(k) + i\epsilon} \right) \right) = \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - \langle \mathbf{k} | (\hat{V} + \hat{V} \frac{1}{\bar{E} - h + i\epsilon} \hat{V}) | \mathbf{k}' \rangle \frac{2i\epsilon}{(E(k') - E(k))^2 + \epsilon^2} \right) \end{aligned} \quad (43)$$

In the limit that $\epsilon \rightarrow 0$

$$\lim_{\epsilon \rightarrow 0^+} \frac{2i\epsilon}{(E(\mathbf{k}') - E(\mathbf{k}))^2 + \epsilon^2} = -2\pi i \delta(E(\mathbf{k}') - E(\mathbf{k})) \quad (44)$$

which implies that (40) becomes

$$\begin{aligned} & \langle \mathbf{P}, \mathbf{k} | S | \mathbf{P}', \mathbf{k}' \rangle = \\ & \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(\mathbf{k}) - E(\mathbf{k}')) \langle \mathbf{k} | (\hat{T}(E - h + i\epsilon) | \mathbf{k}') \rangle \right). \end{aligned} \quad (45)$$

The operator

$$\hat{T}(z) := \hat{V} + \hat{V} \frac{1}{z - h} \hat{V} \quad (46)$$

is called the **transition operator**. Using the second resolvent identities, (42), in (46) shows that $\hat{T}(z)$ is the solution of the integral equations

$$\hat{T}(z) := \hat{V} + \hat{V} \frac{1}{z - h_0} \hat{T}(z) \quad (47)$$

$$\hat{T}(z) = \hat{V} + \hat{T}(z) \frac{1}{z - h_0} \hat{V}. \quad (48)$$

These are called **Lippmann-Schwinger equations** for the transition operator. For scattering theory $z = E + i\epsilon = \frac{\mathbf{k}^2}{2\mu} + i\epsilon$.

The main results of this section can be summarized by the following equations:

$$\begin{aligned} P &= |\langle \Psi^+ | \Psi^- \rangle|^2 \\ \langle \Psi^+ | \Psi^- \rangle &= \langle \Psi_0^+ | S | \Psi_0^- \rangle = \\ & \int \langle \Psi_0^+ | \mathbf{k}, \mathbf{P} \rangle d\mathbf{k} d\mathbf{P} \langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle d\mathbf{k}' d\mathbf{P}' \langle \mathbf{k}', \mathbf{P}' | \Psi_0^- \rangle \end{aligned} \quad (49)$$

with

$$\begin{aligned} & \langle \mathbf{k}, \mathbf{P} | S | \mathbf{k}', \mathbf{P}' \rangle = \\ & \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(\mathbf{k}) - E(\mathbf{k}')) \langle \mathbf{k} | \hat{T}(E + i\epsilon) | \mathbf{k}' \rangle \right) \end{aligned} \quad (50)$$

and

$$\hat{T}(E + i\epsilon) = \hat{V} + \hat{V} \frac{1}{E - h_0 + i\epsilon} \hat{T}(E + i\epsilon). \quad (51)$$

Calculation of the scattering operator using the interaction picture:

The scattering operator can be expressed as

$$S := \Omega_+^\dagger \Omega_- = \lim_{t \rightarrow \infty, t' \rightarrow -\infty} e^{iH_0 \frac{t}{\hbar}} e^{-iH \frac{(t-t')}{\hbar}} e^{-iH_0 \frac{t'}{\hbar}} = \lim_{t \rightarrow \infty, t' \rightarrow -\infty} U_I(t, t') \quad (52)$$

where $U_I(t, -t)$ is the interaction picture time-evolution operator. It satisfies

$$i\hbar \frac{d}{dt} U_I(t, t') = V_I(t) U_I(t, t') \quad U_I(t', t') = I \quad (53)$$

where

$$V_I(t) = e^{\frac{iH_0 t}{\hbar}} V e^{-\frac{iH_0 t}{\hbar}} \quad (54)$$

is the interaction picture interaction. The formal solution can be obtained by iterating the integrated form of (53)

$$U(t, t') = I - \frac{i}{\hbar} \int_{t'}^t V_I(t'') U(t'', t') dt'' \quad (55)$$

The formal solution of this equation is

$$S = I + \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^{\infty} T(V_I(t_1) \cdots V_I(t_n)) dt_1 \cdots dt_n =: \\ T \exp \left(-\frac{i}{\hbar} \int_{-\infty}^{\infty} V_I(t') dt' \right) \quad (56)$$

which is expressed as a time-ordered exponential, where

$$T(V_I(t_1) \cdots V_I(t_n)) = \begin{cases} V_I(t_1) \cdots V_I(t_n) & t_1 > t_2 > \cdots > t_n \\ 0 & \text{otherwise} \end{cases}$$

This is obtained by replacing the n -nested integrals by $n!$ identical integrals obtained by $n!$ permutations of the labels of the integration variables.

This method was used by Dyson to construct S perturbatively in quantum field theory. This series does not necessarily converge even for bounded potentials because the time limits are infinite. Note however that the infinite limits can be replaced by $[-T, T]$ and the result should be unchanged as long as T is large enough. In this case the series with bounded potentials converges because it is bound by the exponential series $e^{2T\|V\|/\hbar}$.

For finite T it is impossible to distinguish bound states from long-lived resonances. If there are bound states the series diverges in the $T \rightarrow \infty$ limit. For this reason the Dyson series is not useful for interactions that have bound eigenstates.

Calculation of the scattering operator using the Lippmann-Schwinger equation:

The starting point is the expression of the scattering probability P in terms of the scattering operator, S

$$P = |\langle \Psi_0^+(0) | S | \Phi_0^-(0) \rangle|^2. \quad (57)$$

As discussed previously, for translationally invariant interactions, $[V, \mathbf{P}] = 0$,

$$e^{iHt/\hbar} e^{-iH_0 t/\hbar} = e^{iht/\hbar} e^{-ih_0 t/\hbar}. \quad (58)$$

This means that when we compute the Møller operators for a translationally invariant potential the total momentum dependence-factors out of all of the matrix elements. This means that

$$\langle \mathbf{P}, \mathbf{k} | \Omega^\pm | \mathbf{P}', \mathbf{k}' \rangle = \delta(\mathbf{P} - \mathbf{P}') \langle \mathbf{k} | \hat{\Omega}^\pm | \mathbf{k}' \rangle \quad (59)$$

where

$$\hat{\Omega}^\pm = \lim_{t \rightarrow \pm\infty} e^{iht/\hbar} e^{-ih_0 t/\hbar}. \quad (60)$$

The scattering eigenstates are defined as

$$|\mathbf{k}^\pm\rangle = \hat{\Omega}^\pm |\mathbf{k}\rangle. \quad (61)$$

The intertwining properties, which for $\hat{\Omega}_\pm$ have the form

$$\hbar \hat{\Omega}_\pm = \hat{\Omega}_\pm h_0 \quad (62)$$

imply that $|\mathbf{k}^\pm\rangle$ are eigenstates of \hbar with energy $\frac{k^2}{2\mu}$:

$$\hbar |\mathbf{k}^\pm\rangle = \hbar \hat{\Omega}^\pm |\mathbf{k}\rangle = \hat{\Omega}^\pm h_0 |\mathbf{k}\rangle = \frac{k^2}{2\mu} \hat{\Omega}^\pm |\mathbf{k}\rangle = \frac{k^2}{2\mu} |\mathbf{k}^\pm\rangle. \quad (63)$$

These solutions are related to the scattering probability by

$$P = |\langle \Psi^+(0) | \Psi^-(0) \rangle|^2 \quad (64)$$

where

$$\langle \mathbf{P}, \mathbf{k} | \Psi^\pm(0) \rangle = \int \langle \mathbf{k} | \mathbf{k}^\pm \rangle d\mathbf{k}' \langle \mathbf{P}, \mathbf{k} | \Psi_0^\pm(0) \rangle. \quad (65)$$

The **time-independent scattering states** are defined by

$$\begin{aligned} |\mathbf{k}^\pm\rangle &:= \lim_{t \rightarrow \pm\infty} e^{-iht/\hbar} e^{ih_0 t/\hbar} |\mathbf{k}\rangle = \\ &(I + \lim_{t \rightarrow \pm\infty} \int_0^t \frac{d}{dt} e^{-iht/\hbar} e^{ih_0 t/\hbar} |\mathbf{k}\rangle. \end{aligned} \quad (66)$$

If the wave packet is included (66) becomes

$$|\psi_0^\pm\rangle + \lim_{t \rightarrow \pm\infty} \int_0^t \frac{d}{dt} \int d\mathbf{k} e^{iht/\hbar} e^{-ih_0 t/\hbar} |\mathbf{k}\rangle \psi_0^\pm(\mathbf{k}). \quad (67)$$

As long as the \mathbf{k} integral is done first the above is equal to

$$|\psi_0^\pm\rangle + \lim_{\epsilon \rightarrow 0} \int_0^{\pm\infty} e^{\mp\epsilon t} \frac{d}{dt} \int d\mathbf{k} (e^{iht/\hbar} e^{-ih_0 t/\hbar}) |\mathbf{k}\rangle \psi_0^\pm(\mathbf{k}). \quad (68)$$

However, when the factor ϵ is included the result is independent of the order of the t and \mathbf{k} integrals. The scattering eigenstate $|\mathbf{k}^\pm\rangle$ can be calculated by

performing the time integral first, with the understanding that the integral must eventually be integrated against a wave packet before taking the $\epsilon \rightarrow 0$ limit..

It follows that the integral in (66) becomes

$$\begin{aligned}
|\mathbf{k}^\pm\rangle &= \\
|\mathbf{k}\rangle + \lim_{\epsilon \rightarrow 0} \int_0^{\pm\infty} e^{\mp\epsilon t} \frac{d}{dt} (e^{iht/\hbar} e^{-ih_0 t/\hbar}) |\mathbf{k}\rangle dt &= \\
|\mathbf{k}\rangle - \lim_{\epsilon \rightarrow 0} \left(\frac{i}{\hbar}\right) \int_0^{\pm\infty} e^{\mp\epsilon t} e^{iht/\hbar} \hat{V} e^{-ih_0 t/\hbar} |\mathbf{k}\rangle dt &= \\
|\mathbf{k}\rangle - \lim_{\epsilon \rightarrow 0} \left(\frac{i}{\hbar}\right) \int_0^{\pm\infty} e^{i(h-E(k)\pm i\epsilon)t/\hbar} \hat{V} |\mathbf{k}\rangle dt &= \\
|\mathbf{k}\rangle + \lim_{\epsilon \rightarrow 0} \frac{1}{E(k) - h \mp i\epsilon} \hat{V} |\mathbf{k}\rangle &=
\end{aligned} \tag{69}$$

where $E(k) = \frac{\mathbf{k}^2}{2\mu}$

This gives the following expression for the scattering eigenstates

$$|\mathbf{k}^\pm\rangle = (I + \frac{1}{E(k) - h \pm i\epsilon} \hat{V}) |\mathbf{k}\rangle \tag{70}$$

The operator

$$\frac{1}{z - h} \tag{71}$$

is the **resolvent** of h . It can be constructed by solving an integral equation. The integral equation can be derived using the **second Resolvent identities**

$$\frac{1}{z - h} - \frac{1}{z - h_0} = \frac{1}{z - h_0} V \frac{1}{z - h} = \frac{1}{z - h} V \frac{1}{z - h_0}. \tag{72}$$

Using these identities in equation (70) with $z = E(k) \pm i\epsilon$ gives

$$\begin{aligned}
|\mathbf{k}^\pm\rangle &= \\
(I + \frac{1}{E(k) - h \pm i\epsilon} \hat{V}) |\mathbf{k}\rangle &= \\
(I + \frac{1}{E(k) - h_0 \pm i\epsilon} \hat{V} \underbrace{(I + \frac{1}{E(k) - h \pm i\epsilon} \hat{V})}_{|\mathbf{k}^\pm\rangle}) |\mathbf{k}\rangle &= \\
|\mathbf{k}\rangle + \frac{1}{E(k) - h_0 \pm i\epsilon} \hat{V} |\mathbf{k}^\pm\rangle &=
\end{aligned} \tag{73}$$

which is called the **Lippmann-Schwinger** equation. It is equivalent to the Schrödinger equation with the asymptotic initial conditions

$$|\mathbf{k}^\pm\rangle = |\mathbf{k}\rangle + (\frac{\mathbf{k}^2}{2\mu} \mp i\epsilon - h_0)^{-1} \hat{V} |\mathbf{k}^\pm\rangle. \tag{74}$$

Unlike the Dyson series it can be used to compute scattering observables when the Hamiltonian has bound states. This equation can be expressed in a coordinate or momentum basis

$$\langle \mathbf{r} | \mathbf{k}^\pm \rangle = \langle \mathbf{r} | \mathbf{k} \rangle + \int \langle \mathbf{r} | (\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{h}_0)^{-1} | \mathbf{r}' \rangle d\mathbf{r}' \hat{V}(\mathbf{r}') \langle \mathbf{r}' | \mathbf{k}^\pm \rangle, \quad (75)$$

$$\langle \mathbf{k}' | \mathbf{k}^\pm \rangle = \langle \mathbf{k}' | \mathbf{k} \rangle + \int (\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \frac{\mathbf{k}''^2}{2\mu})^{-1} \langle \mathbf{k}' | \hat{V} | \mathbf{k}'' \rangle d\mathbf{k}'' \langle \mathbf{k}'' | \mathbf{k}^\pm \rangle. \quad (76)$$

In the coordinate-space basis the free Green functions (matrix elements of the resolvent operator) can be evaluated using the residue theorem. The result of this calculations is

$$\begin{aligned} \langle \mathbf{r} | (\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{h}_0)^{-1} | \mathbf{r}' \rangle &= \frac{1}{(2\pi\hbar)^3} \int d\mathbf{k}' \frac{2\mu e^{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')/\hbar}}{\mathbf{k}^2 - \mathbf{k}'^2 \mp \epsilon} = \\ &= -\frac{\mu}{2\pi\hbar^2} \frac{e^{\pm i k |\mathbf{r} - \mathbf{r}'|/\hbar}}{|\mathbf{r} - \mathbf{r}'|}. \end{aligned} \quad (77)$$

Multiplying (73) by \hat{V} and comparing to (46) gives

$$\hat{V} | \mathbf{k}^\pm \rangle = \hat{V} | \mathbf{k} \rangle + \hat{V} \frac{1}{E(k) - h \mp i\epsilon} \hat{V} | \mathbf{k} \rangle = \hat{T}(E \mp i\epsilon) | \mathbf{k} \rangle \quad (78)$$

It follows that the scattering states, $|\mathbf{k}^\pm\rangle$, can be expressed in terms of the plane wave states, $|\mathbf{k}\rangle$ and the **transition operator**, $\hat{T}(z)$:

$$|\mathbf{k}^\pm\rangle = |\mathbf{k}\rangle + (\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{h}_0)^{-1} \hat{T}(\frac{\mathbf{k}^2}{2\mu} \mp i0^+) |\mathbf{k}\rangle \quad (79)$$

The second resolvent identities can be used to demonstrate the equivalence of the following quantities

$$\langle \mathbf{k}^{+'} | \hat{V} | \mathbf{k} \rangle = \langle \mathbf{k}' | \hat{V} | \mathbf{k}^- \rangle = \langle \mathbf{k}' | \hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0^+) | \mathbf{k} \rangle \quad (80)$$

any of these can be used to calculate plane wave matrix elements of the scattering operator

$$\begin{aligned} \langle \mathbf{P}, \mathbf{k} | S | \mathbf{P}', \mathbf{k}' \rangle &= \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k} | \hat{T}(E - h + i\epsilon) | \mathbf{k}' \rangle \right) &= \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k} | \hat{V} | \mathbf{k}'^- \rangle \right) &= \\ \delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k}^+ | \hat{V} | \mathbf{k}' \rangle \right). \end{aligned} \quad (81)$$

When the potential is weak, $\hat{T}(E - h + i\epsilon) \approx \hat{V}$. This is called the Born approximation. It is justified when

$$\|\hat{V} \frac{1}{E(k) - h_0 \mp i\epsilon}\| \ll 1$$

is small.

An important property of $\hat{T}(z)$ is that it is a short-range operator, like the potential. This means that an approximation to $\hat{T}(z)$ can be found by inserting a complete basis, $\{|n\rangle\}$, in the Lippmann-Schwinger equation and then truncating the sum to a finite number (M) of terms

$$\langle n|\hat{T}(z) \approx \langle n|\hat{V} + \sum_m^M \langle n|\hat{V}(z - \hat{h}_0)^{-1}|m\rangle \langle m|\hat{T}(z) \quad (82)$$

Mathematically the justification for this procedure follows because the kernel of this equation is (normally) a compact operator (on a normed space which may or may not be the Hilbert space). Compactness means that the operator can be *uniformly* approximated by a finite dimensional matrix. Uniformly means that the error of approximating the compact operator C by the finite dimensional matrix M satisfied

$$\|(C - M)|\psi\rangle\| < \epsilon$$

where ϵ is independent of $|\Psi\rangle$, even though $|\Psi\rangle$ is an arbitrary vector in an infinite dimensional Hilbert space. Smaller ϵ require a matrix with a larger dimension.

Eq. (82) is a finite system of linear equations. The solution of this finite system can be used in right-hand side of the Lippmann-Schwinger equation to get an improved approximation to $\hat{T}(z)$:

$$\hat{T}(z) \approx \hat{V} + \sum_m \hat{V}(z - \hat{h}_0)^{-1}|m\rangle \langle m|\hat{T}(z). \quad (83)$$

This improves the convergence and this method is often used in practice.

Scattering cross sections

In a typical experiment the scattering probability, P , is not a useful quantity since the initial and final state vectors are not precisely known. The notion of a scattering cross section is introduced to eliminate the dependence on the choice of wave packets in describing a scattering experiment.

In a real experiment there is an ensemble of beam of particles moving with some mean momentum $\langle \mathbf{p}_b \rangle$ described by a density matrix

$$\rho_b = \sum_n P_{bn} |\phi_{bn}\rangle \langle \phi_{bn}|. \quad \langle \mathbf{p}_b \rangle = \text{Tr}(\mathbf{p}_b \rho_b)$$

These beam particles directed at an ensemble of target particles with mean-momentum $\langle \mathbf{p}_t \rangle$ represented by another density matrix:

$$\rho_t = \sum_m P_{tm} |\phi_{tm}\rangle \langle \phi_{tm}| \quad \langle \mathbf{p}_t \rangle = \text{Tr}(\mathbf{p}_t \rho_t).$$

Typically all of the wave packed in the beam or target will be different in which case P_{bn} and P_{tm} are just one over the number of particles in the beam or target.

Both $\langle \mathbf{p}_b \rangle$ and $\langle \mathbf{p}_t \rangle$ can be measured in an experiment. It is assumed that the target is sufficiently dilute or thin that the probability that a beam particle interacts with more than one target particle is negligibly small. It is also assumed that the interaction between different target particles are sufficiently weak that they can be ignored.

The scattered particles are detected by a detector with a finite resolution. The detector counts any particle that has a momentum directed at the detector within the resolution of the detector. Since charged particles are typically bent by magnets, the particle's that are counted in a given detector depend on both the direction magnitude of the particles mean momentum.

The starting point is to consider a single scattering event. The differential probability of measuring the momenta of final particles 1 and 2 to be within $d\mathbf{p}_1$ of \mathbf{p}_1 and within $d\mathbf{p}_2$ of \mathbf{p}_2 for a given initial asymptotic state $|\Psi_0^-\rangle$ is

$$dP = |\langle \mathbf{p}_1, \mathbf{p}_2 | S | \Psi_0^- \rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2. \quad (84)$$

This is the differential momentum distribution seen after the scattered particles travel beyond the range of the interactions. This change removes any mentions of the final wave packets.

In the absence of scattering $S \rightarrow I$, so that the part of S that causes the scattering is $(S - I)$. Replacing S by $S - I$ in (84) and replacing the single free initial state by the beam and target density matrices gives the differential scattering probability that particles will be detected within $d\mathbf{p}_1$ of \mathbf{p}_1 and $d\mathbf{p}_2$ of \mathbf{p}_2

$$dP = |\langle \mathbf{p}_1, \mathbf{p}_2 | (S - I) | \rho_b \rho_t (S - I)^\dagger | \mathbf{p}_1, \mathbf{p}_2 \rangle| d\mathbf{p}_1 d\mathbf{p}_2 = \sum_{mn} |\langle \mathbf{p}_1, \mathbf{p}_2 | -2\pi i \delta(E_f - E_i) T(E + i0) | \phi_{bn} \phi_{tm} \rangle|^2 P_{bn} P_{tm} d\mathbf{p}_1 d\mathbf{p}_2 \quad (85)$$

Of interest for nuclear and particle physics is the case that the potential is translationally invariant. In this case the matrix elements of $T(z)$ are proportional to $\delta(\mathbf{P}_f - \mathbf{P}_i)$ so the differential probability becomes

$$dP = \sum_{mn} P_{bn} P_{tm} |\langle \mathbf{p}_1, \mathbf{p}_2 | -2\pi i \delta(E_f - E_i) \delta(\mathbf{P}_f - \mathbf{P}_i) \hat{T}(E + i0) | \phi_{bn} \phi_{tm} \rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 = 4\pi^2 \sum_{mn} P_{bn} P_{tm} \int \delta(E_f - E'_i) \delta(E_f - E''_i) \delta(\mathbf{P}'_f - \mathbf{P}'_i) \delta(\mathbf{P}''_f - \mathbf{P}''_i) \times \langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}'_1, \mathbf{p}'_2 \rangle \langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}''_1, \mathbf{p}''_2 \rangle^* \times \phi_{tm}(\mathbf{p}'_1) \phi_{bn}(\mathbf{p}'_2) \phi_{tm}^*(\mathbf{p}''_1) \phi_{bn}^*(\mathbf{p}''_2) d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}'_1 d\mathbf{p}'_2 d\mathbf{p}''_1 d\mathbf{p}''_2 \quad (86)$$

where the integrals are over $\mathbf{p}'_1, \mathbf{p}'_2, d\mathbf{p}''_1$ and \mathbf{p}''_2

The crucial approximation is the assumption that wave functions in the initial beam and target ensembles are sharply peaked around fixed values $\langle \mathbf{p}_b \rangle$ and $\langle \mathbf{p}_t \rangle$ respectively. It is also assumed that T does not change significantly on the scales of momenta where the wave packets are non-zero. This can be controlled in a experiment by reducing the beam dispersion and target temperature.

When the wave packets are not sufficiently sharp, narrow resonance could be washed out, so the it is important to control the momentum dispersion of the beam and target ensembles. For sharply peaked wave functions the following

$$\delta(E_f - E_b - E_t)\delta(E'_i - E''_i)\delta(\mathbf{P} - \langle \mathbf{p}_t \rangle - \langle \mathbf{p}_b \rangle)\delta(\mathbf{P}'_f - \mathbf{P}''_i) \times \\ \langle \mathbf{p}_1, \mathbf{p}_2 | T(E + i0) | \langle \mathbf{p}_t \rangle, \langle \mathbf{p}_b \rangle \rangle \langle \mathbf{p}_1, \mathbf{p}_2 | T(E + i0) | \langle \mathbf{p}_t \rangle, \langle \mathbf{p}_b \rangle \rangle^* \quad (87)$$

Approximating

$$\delta(E_f - E'_i)\delta(E_f - E''_i)\delta(\mathbf{P}'_f - \mathbf{P}'_i)\delta(\mathbf{P}''_f - \mathbf{P}''_i) \\ \langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}'_1, \mathbf{p}'_2 \rangle \langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}''_1, \mathbf{p}''_2 \rangle^* \quad (88)$$

gives

$$dP = \sum_{mn} P_{bn} P_{tm} 4\pi^2 \int \delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\langle \mathbf{p}_t \rangle^2}{2m_t} - \frac{\langle \mathbf{p}_b \rangle^2}{2m_b}\right) \delta(\mathbf{p}_1 + \mathbf{p}_2 - \langle \mathbf{p}_t \rangle - \langle \mathbf{p}_b \rangle) \times \\ |\langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}_t, \mathbf{p}_b \rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 \\ \int \delta(E'_i - E''_i)\delta(\mathbf{P}'_f - \mathbf{P}'_i)\phi_{tm}(\mathbf{p}'_1)\phi_{bn}(\mathbf{p}'_2)\phi_{tm}^*(\mathbf{p}''_1)\phi_{bn}^*(\mathbf{p}''_2)d\mathbf{p}'_1 d\mathbf{p}'_2 d\mathbf{p}''_1 d\mathbf{p}''_2 \quad (89)$$

Representing the delta functions in the integral by

$$\delta(E'_i - E''_i)\delta(\mathbf{P}'_f - \mathbf{P}'_i) = \\ \frac{1}{(2\pi\hbar)^4} e^{i(\mathbf{p}'_1 + \mathbf{p}'_2 - \mathbf{p}''_1 - \mathbf{p}''_2) \cdot \mathbf{x} / \hbar} e^{-i(E'_1 + E'_2 - E''_1 - E''_2)t / \hbar} \cdot \mathbf{x} \quad (90)$$

and observing

$$\phi_{bn}(\mathbf{x}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi_{bn}(\mathbf{p}_b) e^{i\mathbf{p}_b \cdot \mathbf{x} / \hbar - iE_b(\mathbf{p}_b)t} d\mathbf{p}_b \\ \phi_{tm}(\mathbf{x}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \phi_{tm}(\mathbf{p}_t) e^{i\mathbf{p}_t \cdot \mathbf{x} / \hbar - iE_t(\mathbf{p}_t)t} d\mathbf{p}_t, \quad (91)$$

the expression for the differential probability becomes

$$dP = \sum_{mn} P_{bn} P_{tm} 4\pi^2 \int \delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\langle \mathbf{p}_t \rangle^2}{2m_t} - \frac{\langle \mathbf{p}_b \rangle^2}{2m_b}\right) \delta(\mathbf{p}_1 + \mathbf{p}_2 - \langle \mathbf{p}_t \rangle - \langle \mathbf{p}_b \rangle) \times \\ |\langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \langle \mathbf{p}_t \rangle, \langle \mathbf{p}_b \rangle \rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 \\ \frac{(2\pi\hbar)^6}{(2\pi\hbar)^4} |\phi_{tm}(\mathbf{x}, t)|^2 |\phi_{bn}(\mathbf{x}, t)|^2 d\mathbf{x} dt \quad (92)$$

The integral shows that the probability gets contributions from all times when both the n^{th} beam and m^{th} target particles are at the same place. It follows

that the differential probability of a transition per unit time per unit volume into volumes $d\mathbf{p}_1$ and $d\mathbf{p}_2$ about \mathbf{p}_1 and \mathbf{p}_2 is

$$\begin{aligned} \frac{dP}{dVdt} = \sum_{mn} P_{bn} P_{tm} 4\pi^2 \int \delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\langle \mathbf{p}_t \rangle^2}{2m_t} - \frac{\langle \mathbf{p}_b \rangle^2}{2m_b}\right) \delta(\mathbf{p}_1 + \mathbf{p}_2 - \langle \mathbf{p}_t \rangle - \langle \mathbf{p}_b \rangle) \times \\ |\langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \langle \mathbf{p}_t \rangle, \langle \mathbf{p}_b \rangle \rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 \\ \frac{(2\pi\hbar)^6}{(2\pi\hbar)^4} |\phi_{tm}(\mathbf{x}, t)|^2 |\phi_{bn}(\mathbf{x}, t)|^2 \end{aligned} \quad (93)$$

The quantities

$$\sum_m P_{tm} |\phi_{tm}(\mathbf{x}, t)|^2 \quad \text{and} \quad \sum_n P_{bn} |\phi_{bn}(\mathbf{x}, t)|^2 \quad (94)$$

represent the probability density of finding a target and beam particle within $d\mathbf{x}$ of \mathbf{x} at time t .

If we multiply both sides of this equation (94) by the total number of beam and target particles these become the number of beam and target particles per unit volume at \mathbf{x} and time x (recall $P_{tm} \approx 1/N_t$ and $P_{bn} \approx 1/N_b$).

Then $\sum_b N_t P_{bt} \phi_{n0} = n_b(\mathbf{x}, t)$ and $\sum_m N_t P_{mt} \phi_{t0} = n_t(\mathbf{x}, t)$ become the beam and target densities at $d\mathbf{x}$ of \mathbf{x} at time t .

Assume the interactions among different target particles are sufficiently weak that they can be ignored and the target is sufficiently dilute so each particle experiences at most one collision, then we this rate will be proportional to the target density and the number of beam particle crossing a surface per unit time. In this case

$$\begin{aligned} \frac{dN}{dVdt} = d\sigma v_b n_b(\mathbf{x}, t) n_t(\mathbf{x}, t) = v_b \sum_n N_b P_{bn} |\phi_{b0}(\mathbf{x}, t)|^2 \sum_m N_t P_{mt} \phi_{t0}(\mathbf{x}, t)|^2 = \\ N_t N_b \frac{dP}{dVdt} \end{aligned} \quad (95)$$

The proportionality constant, $d\sigma$ is called the **differential cross section** (because it has dimensions of area). Comparing (93) to (95) gives

$$\begin{aligned} d\sigma = \frac{(2\pi)^4 \hbar^2}{v} |\langle \mathbf{p}_1, \mathbf{p}_2 | \hat{T}(E + i0) | \mathbf{p}_t, \mathbf{p}_b \rangle|^2 \times \\ \delta\left(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\mathbf{p}_t^2}{2m_t} - \frac{\mathbf{p}_b^2}{2m_b}\right) \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_t - \mathbf{p}_b) d\mathbf{p}_1 d\mathbf{p}_2 \end{aligned} \quad (96)$$

In using this expression, because of the δ functions, there are 2 independent parameters needed to define the final state. One selects the variables that one chooses to measure in an experiment and integrates over the remaining four variables. This eliminates the delta functions.

One choice is to measure the angular distribution of one particle in the center of momentum frame. In this case integrating over \mathbf{P} eliminates the momentum conserving delta function. The other is eliminated by integrating

$$\int dk k^2 \delta\left(\frac{k^2}{2\mu} + \frac{\mathbf{P}^2}{2M} - E_i\right) = \frac{\mu}{k} \quad (97)$$

The relative velocity of the beam and target is

$$\mathbf{v} = \frac{\mathbf{k}}{m_1} - \frac{-\mathbf{k}}{m_2} = \frac{\mathbf{k}}{\mu} \quad (98)$$

With these substitutions

$$d\sigma_{cm} = (2\pi)^4 \hbar^2 \mu^2 |\langle \mathbf{k}' | \hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0) | \mathbf{k} \rangle|^2 d\hat{\mathbf{k}}' \quad (99)$$

This can be expressed in terms of the **scattering amplitude**

$$d\sigma_{cm} = |F(\mathbf{k}, \mathbf{k}')|^2 d\hat{\mathbf{k}}' \quad (100)$$

where

$$F(\mathbf{k}, \mathbf{k}') := -(2\pi)^2 \mu \hbar \langle \mathbf{k}' | \hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0) | \mathbf{k} \rangle \quad (101)$$

An important property of the transition operator, $\hat{T}(z)$, is its relation to the scattering operator S . We derived it using the formal expression for S :

$$\langle \mathbf{P}', \mathbf{k}' | S | \mathbf{P}, \mathbf{k} \rangle = \delta(\mathbf{P}' - \mathbf{P}) \left(\delta(\mathbf{k}' - \mathbf{k}) - 2\pi i \delta\left(\frac{\mathbf{k}'^2}{2\mu} - \frac{\mathbf{k}^2}{2\mu}\right) \langle \mathbf{k}' | \hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0^+) | \mathbf{k} \rangle \right) \quad (102)$$

Note that we only need $\hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0^+)$, not $\hat{T}(\frac{\mathbf{k}^2}{2\mu} - i0^+)$.

For the laboratory cross section assume that particle 1 is being measured and the target is at rest. Then integrating over the momentum of particle 2 eliminates the 3-momentum conserving delta function. The the energy of the final state is conserved and

$$\langle E_b \rangle = E_f(p_1, \cos(\theta)) = \frac{\mathbf{p}_1^2}{2m_1} + \frac{(\langle \mathbf{p}_b \rangle - \mathbf{p}_1)^2}{2m_2}$$

In this case

$$p_1^2 dp_1 = p_1^2 \frac{dp_1}{dE(p_1)} dE = \frac{p_1^2 dE}{p_1/\mu - \langle p_b \rangle \cos(\theta)/m_2} \quad \mathbf{v} = \frac{\langle \mathbf{p}_b \rangle}{m_b}$$

is used to eliminate the energy integral. In this expression μ is the reduced mass and θ is the scattering angle between the beam direction and \mathbf{p}_1 . In this expression in order to find the angular dependence it is also necessary to express p_1 in terms of the beam energy and the angle θ :

$$p_1 = \frac{m_1 \langle p_b \rangle}{m_1 + m + 2} (\cos(\theta) + \sqrt{\cos^2(\theta) - \frac{m_1^2 - m_2^2}{m_2^2}})$$

This has to be used to express \mathbf{p}_1 in terms of measured quantities. Note that while the angular dependence is different in the center of mass and laboratory coordinate systems, the total cross section invariant.

An important property of the scattering wave function is its structure for very large values of $|\mathbf{r}|$. This turns out to be closely related to the scattering amplitude.

The Lippmann Schwinger equation for the wave function in the coordinate representation is

$$\langle \mathbf{r} | \mathbf{k}^- \rangle = \langle \mathbf{r} | \mathbf{k} \rangle - \frac{\mu}{2\pi\hbar^2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' \hat{V}(\mathbf{r}') \langle \mathbf{r} | \mathbf{k}^- \rangle, \quad (103)$$

For large r this becomes

$$\begin{aligned} \langle \mathbf{r} | \mathbf{k}^- \rangle &\rightarrow \langle \mathbf{r} | \mathbf{k} \rangle - \frac{\mu}{2\pi\hbar^2} \frac{e^{ikr}}{r} e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} d\mathbf{r}' \hat{V}(\mathbf{r}') \langle \mathbf{r} | \mathbf{k}^- \rangle = \\ &\frac{1}{(2\pi\hbar)^{3/2}} (e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} - (2\pi\hbar)^3 \frac{\mu}{2\pi\hbar^2} \frac{e^{\pm ikr}}{r} \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mu k\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}') \langle \mathbf{r}' | \mathbf{k}^\pm \rangle = \\ &\frac{1}{(2\pi\hbar)^{3/2}} (e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} - (2\pi)^2 \hbar \mu \frac{e^{\pm ikr}}{r} \langle \mathbf{k}\hat{\mathbf{r}} | \hat{T}(E + i\epsilon) | \mathbf{k} \rangle) \\ &\frac{1}{(2\pi\hbar)^{3/2}} (e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} + \frac{e^{\pm ikr}}{r} F(k\hat{\mathbf{r}}, \mathbf{k})) \end{aligned}$$

This shows that the scattering amplitude is the amplitude of the scattered wave at a large distance from the scattering center.

Phase shifts

While the scattering operator is the limit of a product of unitary operators, it is not necessarily unitary; however unitarity of S is a physical assumption that is equivalent to the conservation of probability in a scattering experiment. The assume unitarity means that

$$S = e^{2i\delta} \quad (104)$$

In this representation δ is called the phase shift operator. Note that in a basis of energy eigenstates

$$\begin{aligned} \delta(E - E') e^{2i\delta(E)} &= \delta(E - E') (\hat{I} - 2\pi i \langle E | \hat{T}(E + i\epsilon) | E \rangle) = \\ \delta(E - E') (\hat{I} - i \frac{2\pi\mu}{k} \langle \mathbf{k} | \hat{T}(E + i\epsilon) | \mathbf{k} \rangle) \end{aligned} \quad (105)$$

This gives

$$e^{i2\delta(E)} = 1 - i2\pi\mu k \langle \mathbf{k} | \hat{T}(E + i\epsilon) | \mathbf{k} \rangle \quad (106)$$

or

$$e^{i\delta(E)} \sin(\delta(E)) = -\pi\mu k \langle \mathbf{k} | \hat{T}(E + i\epsilon) | \mathbf{k} \rangle =$$

$$\frac{k}{4\pi\hbar} F(\mathbf{k}, \mathbf{k}') \quad (107)$$

For rotationally invariant system the same relations hold for each partial wave; i.e.

$$e^{i\delta_l(E)} \sin(\delta_k(E)) = -\pi\mu k \hat{T}_l(k) \frac{k}{4\pi\hbar} F_l(k) \quad (108)$$

The reason that $\delta_l(k)$ is called a phase shift is because asymptotically the scattering wave in the asymptotic wave function looks like the incoming wave with a shifted phase.

For r larger than the range of the interaction we have

$$\langle r|k^-, l\rangle = \frac{4\pi i^l}{(2\pi\hbar)^{-3/2}} (j_l(kr/\hbar) - \frac{2\mu k i}{\hbar^3} h_l^{(1)}(kr/\hbar) \int_0^\infty j_l(kr'/\hbar) V(r') \langle r'|k^-, l\rangle dr') \quad (109)$$

The integral term is

$$\begin{aligned} \int_0^\infty j_l(kr'/\hbar) V(r') r'^2 dr' \langle r'|k^-, l\rangle &= \frac{(2\pi\hbar)^{3/2}}{4\pi} t_l(k) = \\ &= \frac{(2\pi\hbar)^{3/2}}{4\pi} \left(-1 \frac{1}{\pi k \mu} e^{i\delta_l} \sin(\delta_l)\right) \end{aligned} \quad (110)$$

Inverse scattering

The results of a scattering experiment can be predicted given the Hamiltonian of a the system. The goal of a typical scattering experiment is to verify that the Hamiltonian gives the correct description of the physics. Because of this it is natural to ask if a knowledge of the scattering operator \mathcal{S} is sufficient to determine a unique Hamiltonian. It turns out that the short answer is no. However it is possible to identify necessary and sufficient conditions for two Hamiltonians to give the same scattering operators.

To show this assume that two Hamiltonians H and H' are given. If they equivalent they should have the same spectrum of eigenvalues, which means that they should be related by a unitary transformation, W ,

$$H' = WHW^\dagger. \quad (111)$$

The Møller wave operators for these two Hamiltonians are

$$\Omega_\pm = \lim_{t \rightarrow \pm\infty} e^{iHt} e^{-H_0 t} \quad \text{and} \quad \Omega'_\pm = \lim_{t \rightarrow \pm\infty} e^{iH't} e^{-H_0 t}. \quad (112)$$

It follows that

$$\begin{aligned} \Omega'_\pm &= \\ \lim_{t \rightarrow \pm\infty} e^{iH't} e^{-H_0 t} &= \lim_{t \rightarrow \pm\infty} e^{iWHW^\dagger t} e^{-H_0 t} = W \lim_{t \rightarrow \pm\infty} e^{iHt} W^\dagger e^{-H_0 t} = \\ W \lim_{t \rightarrow \pm\infty} e^{iHt} (I - I + W^\dagger) e^{-H_0 t} &= W \Omega_\pm + \lim_{t \rightarrow \pm\infty} W e^{iHt} (I - W^\dagger) e^{-H_0 t} \end{aligned}$$

The identity

$$\Omega'_\pm = W\Omega_\pm \quad (113)$$

follows provided

$$\begin{aligned} 0 &= \lim_{t \rightarrow \pm\infty} \|W e^{iHt} (I - W^\dagger) e^{-iH_0 t} |\psi\rangle\| = \lim_{t \rightarrow \pm\infty} \|(I - W^\dagger) e^{-iH_0 t} |\psi\rangle\| = \\ &\lim_{t \rightarrow \pm\infty} \|W^\dagger (W - I) e^{-iH_0 t} |\psi\rangle\| = \lim_{t \rightarrow \pm\infty} \|(W - I) e^{-iH_0 t} |\psi\rangle\|. \end{aligned} \quad (114)$$

This condition is a short-range condition on the unitary transformation W . Since this condition only involves H_0 it is independent of H .

If W is unitary and satisfies (114) then

$$S' = \Omega_+^\dagger \Omega'_- = \Omega_+^\dagger W^\dagger W \Omega_- = \Omega_+^\dagger \Omega_- = S$$

This shows that any two Hamiltonians related by a unitary W satisfying (114) give the same scattering operator. Note that even though H and H' are related by a unitary transformation, the H_0 in Ω_\pm and Ω'_\pm is the same. The condition (114) means that

$$H = H_0 + V \quad \text{and} \quad H' = H_0 + V'$$

where both V and V' are short-range interactions.

Unitarity and (114) are sufficient conditions for $S = S'$, it turns out that they are necessary. Specifically if $S = \Omega_+^\dagger \Omega_- = \Omega_+^\dagger \Omega'_- = S'$ then there is a unitary W satisfying (111) and (114).

The simplest case is when both Hamiltonians have no bound states. In that case the Møller wave operators are unitary. Multiplying

$$\Omega_+^\dagger \Omega_- = \Omega_+^\dagger \Omega'_-$$

on the left by Ω'_+ and on the right by Ω_-^\dagger gives

$$\Omega'_+ \Omega_+^\dagger = \Omega'_- \Omega_-^\dagger.$$

It follows from the intertwining condition (15) that

$$\Omega'_\pm \Omega_\pm^\dagger H = \Omega'_\pm H_0 \Omega_\pm^\dagger = H' \Omega'_\pm \Omega_\pm^\dagger$$

which shows

$$W := \Omega'_\pm \Omega_\pm^\dagger \quad (115)$$

satisfies

$$H' = W H W^\dagger$$

In addition it follows from (115) that

$$\Omega'_\pm = W \Omega_\pm$$

which can be written as

$$\begin{aligned}
0 &= \lim_{t \rightarrow \pm\infty} \|(e^{iH't} e^{-H_0 t} - W e^{iHt} e^{-H_0 t})|\psi\rangle\| = 0 = \\
&\lim_{t \rightarrow \pm\infty} \|W(e^{iHt} W^\dagger e^{-H_0 t} - e^{iHt} e^{-H_0 t})|\psi\rangle\| = \\
&\lim_{t \rightarrow \pm\infty} \|(W^\dagger - I)e^{-H_0 t}|\psi\rangle\| = \lim_{t \rightarrow \pm\infty} \|W^\dagger(I - W)e^{-H_0 t}|\psi\rangle\| = \\
&\lim_{t \rightarrow \pm\infty} \|(I - W)e^{-H_0 t}|\psi\rangle\| \lim_{t \rightarrow \pm\infty} \|(W - I)e^{-iH_0 t}|\psi\rangle\| = \\
&\lim_{t \rightarrow \pm\infty} \|e^{iH't}(W - I)e^{-iH_0 t}|\psi\rangle\| \lim_{t \rightarrow \pm\infty} \|(\Omega'_\pm \Omega_\pm^\dagger - I)e^{-iH_0 t}|\psi\rangle\| = \\
&\lim_{t \rightarrow \pm\infty} \|(\Omega_\pm^\dagger - \Omega'_\pm)e^{-iH_0 t}|\psi\rangle\| \tag{116}
\end{aligned}$$

This is for the case that Ω is unitary. When Ω_\pm is not unitary (115) is replaced by

$$W := \Omega'_\pm \Omega_\pm^\dagger + \sum_n |b'_n\rangle\langle b_n|$$

where the sum is over all bound states and $|b_n\rangle, |b'_n\rangle$ are the normalized bound eigenstates of H and H' . In this case in addition to $S = S'$, H and H' must have have the same number of bound states with the same eigenvalues and multiplicities. The proof of the necessary condition follows case when there are no bound states.

An important comment is that the (115) must hold for both time limits. The result is true is there is a different W for each time limit. It is clear the two Hamiltonians with short range repulsive potential do not have the same scattering operator, but because they have the same spectrum they are unitarily equivalent. What fails is that condition (115) is not satisfied for both time limits.

Multi channel scattering:

Let H be the Hamiltonian for a system of N particles with short-range interactions. In general, the Hamiltonian H will have both two-body and many-body interactions. The notation \mathbf{a} denotes a partition of the N particles into n_a non-empty disjoint subsystems, labeled by \mathbf{a}_i , and $H_{\mathbf{a}_i}$ is the part of H involving only the particles in the i^{th} subsystem of the partition \mathbf{a} .

In this section, scattering channels will always be associated with the N -particle system. There is a scattering channel, α , associated with the partition \mathbf{a} if each subsystem Hamiltonian, $H_{\mathbf{a}_i}$, has a bound state or is a single particle Hamiltonian. A bound state associated with $H_{\mathbf{a}_i}$ is denoted by

$$|(E_i, j_i) \mathbf{p}_i, \mu_i\rangle \quad \text{where} \quad 1 \leq i \leq n_a.$$

In this notation, j_i is the total intrinsic angular momentum of the i^{th} bound state, μ_i is the magnetic quantum number of the i^{th} bound state, \mathbf{p}_i is the total momentum of the i^{th} bound state, and

$$E_i = \frac{\mathbf{p}_i^2}{2M_i} - e_{\mathbf{a}_i}$$

is the total kinetic energy minus the binding energy, e_{a_i} , of the i^{th} bound subsystem (M_i is the total mass of the i^{th} bound subsystem). In general, for a given partition, a , of the N particles into n_a subsystems, there may be one or more scattering channels or zero channels associated with the partition a . The notation \mathcal{A} is used to denote the set of all scattering channels of the N -body system, which by convention also includes the one-body channels (N -body bound states). Except for the one-body channels, the set \mathcal{A} of scattering channels is determined by the solution of *proper subsystem problems*.

The notation discussed so far can be illustrated by considering the subsystem Hamiltonians for a seven-particle system associated with the partition $a = (135)(27)(46)$. There is a scattering channel associated with this partition if each of the three subsystem Hamiltonians can form bound states:

$$a = \underbrace{(135)}_{a_1} \underbrace{(27)}_{a_2} \underbrace{(46)}_{a_3} \quad n_a = 3 \quad N = 7 = n_{a_1} + n_{a_2} + n_{a_3}$$

$$H_{a_1} = K_1 + K_3 + K_5 + V_{13} + V_{15} + V_{35} + V_{135}$$

$$H_{a_2} = K_2 + K_7 + V_{27}$$

$$H_{a_3} = K_4 + K_6 + V_{46}$$

$$H_{a_1} |(E_1, j_1) \mathbf{p}_1, \mu_1\rangle = \left(\frac{\mathbf{p}_1^2}{2(m_1 + m_3 + m_5)} - e_{135} \right) |(E_1, j_1) \mathbf{p}_1, \mu_1\rangle$$

where $\mathbf{p}_1 = \mathbf{k}_1 + \mathbf{k}_3 + \mathbf{k}_5$,

$$H_{a_2} |(E_2, j_2) \mathbf{p}_2, \mu_2\rangle = \left(\frac{\mathbf{p}_2^2}{2(m_2 + m_7)} - e_{27} \right) |(E_2, j_2) \mathbf{p}_2, \mu_2\rangle$$

where $\mathbf{p}_2 = \mathbf{k}_2 + \mathbf{k}_7$,

$$H_{a_3} |(E_3, j_3) \mathbf{p}_3, \mu_3\rangle = \left(\frac{\mathbf{p}_3^2}{2(m_4 + m_6)} - e_{46} \right) |(E_3, j_3) \mathbf{p}_3, \mu_3\rangle$$

where $\mathbf{p}_3 = \mathbf{k}_4 + \mathbf{k}_6$, \mathbf{k}_i are the single-particle momenta, K_i are the single-particle kinetic energies, V_{ij} are two-body interactions, V_{135} is a three-body interaction, and e_{135} , e_{27} and e_{46} are the binding energies of the bound states.

For a given scattering channel α , there are scattering states associated with two different asymptotic conditions. The different asymptotic conditions replace the initial conditions of the scattering states with conditions that relate the scattering states in the asymptotic past ($-$) or asymptotic future ($+$) to states of non-interacting bound subsystems. The scattering states, $|\Psi_\alpha^{(\pm)}\rangle$, associated with the channel α are defined by strong limits:

$$\lim_{t \rightarrow \pm\infty} \left\| |\Psi_\alpha^{(\pm)}\rangle - \sum_{\mu_1, \dots, \mu_{n_a}} \int e^{iHt} e^{-iH_a t} \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle \phi_i(\mathbf{p}_i, \mu_i) d\mathbf{p}_i \right\| = 0, \quad (117)$$

where the partition Hamiltonian, H_a , is the sum of subsystem Hamiltonians

$$H_a = \sum_{i=1}^{n_a} H_{a_i} \quad \text{with} \quad H_{a_i} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle = E_i |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle \quad (118)$$

and satisfies

$$H_a \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle = \left(\sum_{q=1}^{n_a} E_q \right) \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle. \quad (119)$$

The operator H_a is the part of the Hamiltonian with all of the interactions between particles in the different clusters of the partition a turned off, and $\phi_i(\mathbf{p}_i, \mu_i)$ are wave packets in the total momentum and magnetic quantum numbers of each bound subsystem in the channel α . The variables in the wave packets are the experimentally detectable degrees of freedom (momentum and spin polarization) of the bound subsystems.

The limit in (117) is a strong limit, and this means that the integral over the wave packets must be computed *before* taking the limit. If this is done in the correct order, then inserting an extra factor of $e^{\mp \epsilon t}$ and taking the limit as $\epsilon \rightarrow 0$ *after* performing the integral does not change the result. This makes it possible to define the limit using “plane wave” states where the $\epsilon \rightarrow 0$ limit can be taken at the end of the calculation *after* integrating against the wave packets. After including the factor of $e^{\mp \epsilon t}$, the channel α scattering states

$$|\Psi_\alpha^{(\pm)}\rangle = \lim_{\epsilon \rightarrow 0} \sum_{\mu_1, \dots, \mu_{n_a}} \int |\Psi_\alpha^{(\pm)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a})\rangle \prod_{i=1}^{n_a} \phi_i(\mathbf{p}_i, \mu_i) d\mathbf{p}_i \quad (120)$$

can be expressed in terms of the channel α “plane wave” scattering states defined by

$$\begin{aligned} |\Psi_\alpha^{(\pm)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a})\rangle &:= \lim_{t \rightarrow \pm\infty} e^{iHt \mp \epsilon t} e^{-iH_a t} \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle = \\ &\otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle + \lim_{t \rightarrow \pm\infty} \int_0^t \frac{d}{dt} (e^{iHt \mp \epsilon t} e^{-iH_a t}) \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle dt = \\ &\otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle \\ &+ i \lim_{t \rightarrow \pm\infty} \int_0^t e^{iHt \mp \epsilon t} (H \pm i\epsilon - H_a) e^{-iH_a t} \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle dt = \\ &\otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle + (E_\alpha - H \mp i\epsilon)^{-1} H^a \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle. \end{aligned} \quad (121)$$

The operator $H^a := H - H_a$ is the sum of interactions between particles in different clusters of a , and

$$E_\alpha = \sum_{q=1}^{n_a} \left(\frac{\mathbf{p}_q^2}{2M_q} - e_{a_q} \right) \quad (122)$$

is the total energy of the system (M_q is the total mass of the q^{th} subsystem). The limit $\epsilon \rightarrow 0$ in (121) can only be taken after integrating against products of wave packets which are functions of the momenta and magnetic quantum numbers of each bound cluster.

The tensor product of the wave packets span a channel Hilbert space \mathcal{H}_α . The operator, Φ_α , that maps the channel α Hilbert space \mathcal{H}_α to the N -body Hilbert space \mathcal{H} is defined by

$$\Phi_\alpha |\phi_{o\alpha}\rangle := \sum_{\mu_1, \dots, \mu_{n_a}} \int \otimes_{i=1}^{n_a} |(E_i, j_i) \mathbf{p}_i, \mu_i\rangle \phi_i(\mathbf{p}_i, \mu_i) d\mathbf{p}_i, \quad (123)$$

where $|\phi_{o\alpha}\rangle \in \mathcal{H}_\alpha$ represents the product of wave packets given by

$$\langle \mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a} | \phi_{o\alpha} \rangle := \prod_{q=1}^{n_a} \phi_q(\mathbf{p}_q, \mu_q). \quad (124)$$

The wave packets describe the experimentally accessible momentum and spin distributions for the reaction. The mapping, $\Phi_\alpha : \mathcal{H}_\alpha \rightarrow \mathcal{H}$, is called the channel injection operator, and it includes the internal variables of the bound state wave functions for each bound subsystem. In this two-Hilbert space notation, the channel α “plane wave” scattering states are expressed in terms of channel wave operators:

$$|\Psi_\alpha^{(\pm)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a})\rangle = \lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_a t} \Phi_\alpha = \Omega^{(\pm)}(a) \Phi_\alpha \quad (125)$$

where

$$\Omega^{(\pm)}(a) := \lim_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_a t} \quad (126)$$

only makes sense as a strong limit applied to the normalizable vector $\Phi_\alpha |\phi_{o\alpha}\rangle$. The advantage of the notation in (??) is that it separates the part of the scattering state that depends on the partition a from the part that depends on the associated scattering channel α . The operators $\Omega^{(\pm)}(a)$ act on the N -body Hilbert space, while Φ_α acts on the degrees of freedom that can be measured in an experiment.

The probability amplitude density for a transition from an initial channel state α to a final channel state β (the scattering matrix) is

$$\begin{aligned} \langle \Psi_\beta^{(+)}(\mathbf{p}'_1, \mu'_1, \dots, \mathbf{p}'_{n_b}, \mu'_{n_b}) | \Psi_\alpha^{(-)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a}) \rangle = \\ \langle \beta, \mathbf{p}'_1, \mu'_1, \dots, \mathbf{p}'_{n_b}, \mu'_{n_b} | S_{\beta\alpha} | \alpha, \mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a} \rangle, \end{aligned} \quad (127)$$

where the channel scattering operator, $S_{\beta\alpha} := \Phi_\beta^\dagger \Omega^{(+)\dagger}(b) \Omega^{(-)}(a) \Phi_\alpha$, is used to express the scattering matrix in terms of the non-interacting bound subsystems in the channels α and β (the channel β is associated with the partition b). The channel scattering operator, $S_{\beta\alpha}$, is a mapping from \mathcal{H}_α to \mathcal{H}_β . The channel Hilbert spaces are spaces of square integrable functions of the experimentally observable degrees of freedom in each scattering channel.

In a scattering process, the incoming $(-)$ states look like free bound clusters long before the collision, and the outgoing $(+)$ states look like free bound clusters long after the collision. Since there can be scattering from the channel α to the channel β , the incoming and outgoing scattering states for different channels with different asymptotic conditions (\pm) are not orthogonal; however, the scattering states for different channels with the same asymptotic condition (\pm) are orthogonal and complete if the bound state channels are included. This assumes that the theory is asymptotically complete, which is an assumption that the original Hamiltonian is not pathological.

While the scattering matrix is the inner product of states satisfying incoming $(-)$ and outgoing $(+)$ asymptotic conditions, it can be expressed in terms of only the incoming scattering states

$$|\Psi_{\alpha}^{(-)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a})\rangle.$$

This is because $\Omega^{(+)\dagger}(a)$ and $\Omega^{(-)}(a)$ both involve limits of e^{-iHt} with $t \rightarrow +\infty$. While the scattering matrix elements could also be expressed in terms of states with the $(+)$ asymptotic condition, in both cases $t \rightarrow +\infty$ is a preferred direction of time evolution in scattering reactions.

The resulting expression for scattering matrix elements is

$$\begin{aligned} \langle \beta, \mathbf{p}'_1, \mu'_1, \dots, \mathbf{p}'_{n_b}, \mu'_{n_b} | S_{\beta\alpha} | \alpha, \mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a} \rangle = \\ \delta_{\beta\alpha} \prod_i \delta(\mathbf{p}'_i - \mathbf{p}_i) \delta_{\mu'_i \mu_i} \\ - 2\pi i \delta(E'_\beta - E_\alpha) \langle \mathbf{p}'_1, \mu'_1, \dots, \mathbf{p}'_{n_b}, \mu'_{n_b} | \Phi_\beta^\dagger H^b | \Psi_{\alpha}^{(-)}(\mathbf{p}_1, \mu_1, \dots, \mathbf{p}_{n_a}, \mu_{n_a}) \rangle, \end{aligned} \quad (128)$$

where $H^b := H - H_b$ is the part of H that only has interactions between particles in different clusters of b . For short-range interactions, the operator H^b will vanish as the clusters of b are asymptotically separated. Equation (128) can be expressed in operator form using the notation in (125):

$$S_{\beta\alpha} = I\delta_{\beta\alpha} - 2\pi i \delta(E'_\beta - E_\alpha) \Phi_\beta^\dagger H^b \Omega^{(-)}(a) \Phi_\alpha, \quad (129)$$

where

$$T^{\beta\alpha} := \Phi_\beta^\dagger H^b \Omega^{(-)}(a) \Phi_\alpha \quad (130)$$

is the right half-shell transition matrix element. The presence of the energy conserving delta function $\delta(E'_\beta - E_\alpha)$ ensures that the scattering matrix is only defined for *on-shell* values of the energy.

Assuming that the Hamiltonian commutes with the total linear momentum, the differential cross section for scattering from a 2-cluster channel α to a general channel β can be expressed in terms of the above quantities as

$$\begin{aligned} d\sigma = \frac{(2\pi)^4}{|s \mathbf{v}_r|} |\langle \mathbf{p}'_1, \mu'_1, \dots, \mathbf{p}'_{n_b}, \mu'_{n_b} | \Phi_\beta^\dagger H^b \Omega^{(-)}(a) \Phi_\alpha | \mathbf{p}_1, \mu_1, \mathbf{p}_2, \mu_2 \rangle|^2 \\ \times \delta\left(\sum_{j=1}^{n_b} E'_j - E_1 - E_2\right) \delta\left(\sum_{j=1}^{n_b} \mathbf{p}'_j - \mathbf{p}_1 - \mathbf{p}_2\right) \prod_{i=1}^{n_b} d\mathbf{p}'_i. \end{aligned} \quad (131)$$

In the above expression, \mathbf{v}_r is the relative velocity of the incoming pair of particles and $s = \prod_q k_q!$ is a statistical normalization factor for identical bound states in the final state, with k_q denoting the number of identical bound states of type q in the final state. In (131), the $\|\cdots\|$ indicates that a momentum conserving delta function has been factored out of the expression so that

$$\langle \mathbf{p}'_1, \mu'_1, \cdots, \mathbf{p}'_{n_b}, \mu'_{n_b} | \Phi_\beta^\dagger H^b \Omega^{(-)}(a) \Phi_\alpha | \mathbf{p}_1, \mu_1, \mathbf{p}_2, \mu_2 \rangle = \delta\left(\sum_{j=1}^{n_b} \mathbf{p}'_j - \mathbf{p}_1 - \mathbf{p}_2\right) \langle \mathbf{p}'_1, \mu'_1, \cdots, \mathbf{p}'_{n_b}, \mu'_{n_b} \| \Phi_\beta^\dagger H^b \Omega^{(-)}(a) \Phi_\alpha \| \mathbf{p}_1, \mu_1, \mathbf{p}_2, \mu_2 \rangle. \quad (132)$$

The differential cross section in (131) contains several independent variables, but in an experiment one chooses the variables that will be measured and integrates over the remaining variables in order to eliminate the delta functions. The differential cross section is only defined for *on-shell* matrix elements.

Spin dependent scattering

More details about the Hamiltonian can be extracted by considering the spin dependence of the cross section. The formula for the cross section is an idealization with respect to the polarizations. No experiment has perfectly polarized targets, beams or can perfectly identify polarizations in detectors. The uncertainties can be treated using spin density matrices.

We assume that the polarizations in the target and beam have a classical probability distribution given by the density matrices

$$\rho_b := |\mu_b\rangle P_{b\mu_b} \langle \mu_b| \times I_t \quad (133)$$

$$\rho_t := |\mu_t\rangle P_{t\mu_t} \langle \mu_t| \times I_b \quad (134)$$

where $P_{b\mu_b}$ and $P_{t\mu_t}$ represent the classical probability for a particle in the beam (target) to have spin polarization μ_b (μ_t). Averaging over initial over initial spin and target states gives

$$\begin{aligned} d\sigma = \sum_{\mu_b \mu_t} \frac{(2\pi)^4}{vs} \langle \mathbf{p}_1, \mu_1 \cdots, \mathbf{p}_n, \mu_n \| T^{\alpha\beta} \| \bar{\mathbf{p}}_b, \mu_b, \bar{\mathbf{p}}_t, \mu_t \rangle \rho_{b\mu_b \mu_b} \rho_{t\mu_t \mu_t} \times \\ \langle \bar{\mathbf{p}}_b, \mu_b, \bar{\mathbf{p}}_t, \mu_t \| T^{\alpha\beta\dagger} \| \mathbf{p}_1, \mu_1 \cdots, \mathbf{p}_n, \mu_n \rangle \times \\ \delta(\langle \mathbf{p}_b \rangle + \langle \mathbf{p}_t \rangle - \sum_{i=1}^N \mathbf{p}_i) \delta(E_b + E_t - \sum_{i=1}^N E_i) \prod_{i=1}^N d\mathbf{p}_i. \end{aligned} \quad (135)$$

In this expression there are

In these expression we chose spin bases where the density matrices are diagonal; in general the density matrices are Hermitian matrices with unit trace. In a general spin basis the above expression is replaced by

$$\begin{aligned}
d\sigma = \sum_{\mu_b \mu_t} \frac{(2\pi)^4}{vs} \langle \mathbf{p}_1, \mu_1 \cdots, \mathbf{p}_n, \mu_n \| T^{\alpha\beta} \| \bar{\mathbf{p}}_b, \mu_b, \bar{\mathbf{p}}_t, \mu_t \rangle \rho_{b\mu_b \mu'_b} \rho_{t\mu_t \mu'_t} \times \\
\langle \bar{\mathbf{p}}_b, \mu'_b, \bar{\mathbf{p}}_t, \mu'_t \| T^{\alpha\beta\dagger} \| \mathbf{p}_1, \mu_1 \cdots, \mathbf{p}_n, \mu_n \rangle \times \\
\delta(\langle \mathbf{p}_b \rangle + \langle \mathbf{p}_t \rangle - \sum_{i=1}^N \mathbf{p}_i) \delta(E_b + E_t - \sum_{i=1}^N E_i) \prod_{i=1}^N d\mathbf{p}_i. \quad (136)
\end{aligned}$$

It is useful to define the matrix

$$\langle \mu_1, \mu_2, \cdots, \mu_n \| T \mu_b, \mu_t \rangle$$

In this notation the differential cross section becomes

$$\begin{aligned}
d\sigma = \sum_{\mu_b \mu_t} \frac{(2\pi)^4}{vs} T^\dagger \rho_b \rho_t T \delta(\langle \mathbf{p}_b \rangle + \langle \mathbf{p}_t \rangle - \sum_{i=1}^N \mathbf{p}_i) \delta(E_b + E_t - \sum_{i=1}^N E_i) \times \\
\prod_{i=1}^N d\mathbf{p}_i \cdot \langle \mathbf{p}_1, \mu_1 \cdots, \mathbf{p}_n, \mu_n \| T^{\alpha\beta} \| \bar{\mathbf{p}}_b, \mu_b, \bar{\mathbf{p}}_t, \mu_t \rangle
\end{aligned}$$

The quantity is diagonal in the final spin indices, however just like in the case of the initial spins, it will not be diagonal in a general spin basis. There are $((2j_1 + 1) \cdots (2j_n + 1))^2 = N^2$ possible combinations of final spin indices. Computationally the final state information can be encoded in a final state density matrix. This is normally treated by constructing a basis of independent $N \times N$ Hermitian matrices S_i with the property

$$\text{Tr}(S_i S_j) = \delta_{ij} \quad (137)$$

General polarization observables can be computed using

$$P^i = \frac{\text{Tr}(S^i T \rho_t \rho_b T^\dagger)}{\text{Tr}(T \rho_t \rho_b T^\dagger)} \quad (138)$$

which is the ratio of the S_i polarized cross section to the cross section summed over all final spin states. In this notation a general polarization observable can be computed as

$$\langle O \rangle = \frac{\text{Tr}(O T \rho_t \rho_b T^\dagger)}{\text{Tr}(T \rho_t \rho_b T^\dagger)} = \text{Tr}(O S^i) P^i. \quad (139)$$

1 Two potential scattering

When the Hamiltonian is a linear combination of an interaction that must be treated non-perturbatively one that can be treated perturbatively it is useful to use the two-potential formalism of Gell-Mann and Goldberger. To illustrate how this works assume a Hamiltonian of the form

$$H = H_0 + V_s + V_w \quad (140)$$

where V_s is strong and V_w is weak. First consider the case of two-body scattering where both interactions are short-range interactions. In this H_0 is the asymptotic Hamiltonian and the scattering operator can be expressed as

$$S = \lim_{t \rightarrow \infty} e^{iH_0 t} e^{-2iHt} e^{iH_0 t} = \lim_{t \rightarrow \infty} e^{iH_0 t} e^{-i(H_0 + V_s)t} e^{i(H_0 + V_s)t} e^{-2iHt} e^{i(H_0 + V_s)t} e^{-i(H_0 + V_s)t} e^{iH_0 t}. \quad (141)$$

This can be replaced by the product of three limits

$$\lim_{t \rightarrow \infty} e^{iH_0 t} e^{-i(H_0 + V_s)t} \lim_{t \rightarrow \infty} e^{i(H_0 + V_s)t} e^{-2iHt} e^{i(H_0 + V_s)t} \lim_{t \rightarrow \infty} e^{-i(H_0 + V_s)t} e^{iH_0 t} \quad (142)$$

This is valid if all three limits exist. This gives

$$S = \Omega_+^\dagger(H_0 + V_s, H_0) \lim_{t \rightarrow \pm\infty} e^{i(H_0 + V_s)t} e^{-2iHt} e^{i(H_0 + V_s)t} \Omega_-(H_0 + V_s, H_0). \quad (143)$$

Since V_w is weak it can be treated by perturbation theory. To do this define interaction picture evolution operator

$$U(t, t') = e^{i(H_0 + V_s)t} e^{-iH(t-t')} e^{-i(H_0 + V_s)t'}. \quad (144)$$

$U(t, t')$ the solution of the integral equation

$$U(t, t') = I - i \int_{t'}^t V_W(t'') U(t'', t') dt'' \quad V_W(t) := e^{i(H_0 + V_s)t} V_W e^{-i(H_0 + V_s)t}. \quad (145)$$

Using the Dyson trick to remove the iterated integrals the iterative solution of this equation can be expressed as a series of time ordered products of $V_W(t)$ integrated over a single time interval:

$$U(t, t') = I + \sum_n \frac{(-i)^n}{n!} \int_{t'}^t dt_1 \cdots dt_n T(V_W(t_1) \cdots V_W(t_n)) \quad (146)$$

where T is the time ordering operator. To use this in (145) let $t \rightarrow \infty$, $t' \rightarrow -\infty$ which gives the following expression for the scattering operator

$$S = \Omega_+^\dagger(H_0 + V_s, H_0) \times$$

$$[I + \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots dt_n T(V_W(t_1) \cdots V_W(t_n))] \Omega_-(H_0 + V_s, H_0) \quad (147)$$

The leading three terms in this perturbative series for the scattering operator are

$$\begin{aligned} S &= \Omega_+^\dagger(H_0 + V_s, H_0) \Omega_-(H_0 + V_s, H_0) \\ &- i \int_{-\infty}^{\infty} dt_1 \Omega_+^\dagger(H_0 + V_s, H_0) V_w(t_1) \Omega_-(H_0 + V_s, H_0) \\ &- \frac{1}{2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \Omega_+^\dagger(H_0 + V_s, H_0) \times \\ &[V_W(t_1) V_W(t_2) \theta(t_1 - t_2) + V_W(t_2) V_W(t_1) \theta(t_2 - t_1) + \cdots] \\ &\Omega_-(H_0 + V_s, H_0). \end{aligned} \quad (148)$$

Expanding in eigenstates of $H_0 + V_s$ and using the representation for the Heaviside function,

$$\theta(t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{ds e^{ist}}{s - i\epsilon^+}, \quad (149)$$

gives

$$\begin{aligned} S &= \sum_n \Omega_+^\dagger(H_0 + V_s, H_0) |n\rangle \langle n| \Omega_-(H_0 + V_s, H_0) \\ &- i \sum_{nm} \int_{-\infty}^{\infty} dt_1 \Omega_+^\dagger(H_0 + V_s, H_0) |n\rangle e^{i(E_n - E_m)t_1} \langle n| V_w |m\rangle \langle m| \Omega_-(H_0 + V_s, H_0) \\ &- \frac{1}{2} \sum_{mnk} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \Omega_+^\dagger(H_0 + V_s, H_0) |n\rangle [\langle n| V_w |k\rangle \langle k| V_w |m\rangle \times \\ &e^{i(E_n - E_k)t_1} e^{i(E_k - E_m)t_2} \theta(t_1 - t_2) + \\ &\langle n| V_w |k\rangle \langle k| V_w |m\rangle e^{i(E_n - E_k)t_2} e^{i(E_k - E_m)t_1} \theta(t_2 - t_1) + \cdots] \\ &\langle m| \Omega_-(H_0 + V_s, H_0) + \cdots \end{aligned} \quad (150)$$

This gives

$$\begin{aligned} S &= \Omega_+^\dagger(H_0 + V_s, H_0) \Omega_-(H_0 + V_s, H_0) \\ &- i 2\pi \delta(E_f - E_i) \Omega_+^\dagger(H_0 + V_s, H_0) V_w \Omega_-(H_0 + V_s, H_0) \\ &- \frac{1}{2} \sum_{mnk} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} ds \Omega_+^\dagger(H_0 + V_s, H_0) |n\rangle [\langle n| V_w |k\rangle \langle k| V_w |m\rangle \times \\ &e^{i(E_n - E_k)t_1} e^{i(E_k - E_m)t_2} \frac{e^{is(t_1 - t_2)}}{(2\pi i)(s - i\epsilon)} \\ &+ \langle n| V_w |k\rangle \langle k| V_w |m\rangle e^{i(E_n - E_k)t_2} e^{i(E_k - E_m)t_1} \frac{e^{is(t_2 - t_1)}}{(2\pi i)(s - i\epsilon)}] \langle m| \Omega_-(H_0 + V_s, H_0) + \cdots = \end{aligned} \quad (151)$$

$$\begin{aligned}
S &= \Omega_+^\dagger(H_0 + V_s, H_0)\Omega_-(H_0 + V_s, H_0) \\
&\quad - i2\pi\delta(E_f - E_i)\Omega_+^\dagger(H_0 + V_s, H_0)V_w\Omega_-(H_0 + V_s, H_0)] \\
&\quad - \frac{2}{2} \frac{(2\pi)^2}{2\pi i} \sum_{mnk} \delta(E_n - E_m)\Omega_+^\dagger(H_0 + V_s, H_0)|n\rangle \left[\frac{\langle n|V_w|k\rangle\langle k|V_w|m\rangle}{(2\pi i)(E_k - E_m - i\epsilon)} \Omega_-(H_0 + V_s, H_0) \right. \\
&\quad \left. \right] \tag{152}
\end{aligned}$$

$$\begin{aligned}
S &= \Omega_+^\dagger(H_0 + V_s, H_0)\Omega_-(H_0 + V_s, H_0) \\
&\quad - i2\pi\delta(E_f - E_i)\Omega_+^\dagger(H_0 + V_s, H_0)V_W\Omega_-(H_0 + V_s, H_0)] \\
&\quad - 2\pi i\delta(E_f - E_i)\Omega_+^\dagger(H_0 + V_s, H_0)V_W \frac{1}{E_i - H_0 - V_s + i\epsilon} V_W\Omega_-(H_0 + V_s, H_0) + \dots \\
&\quad \tag{153}
\end{aligned}$$

This is exactly the second Born approximation in the strongly interacting eigenstates.

For the multi-channel case it is enough to replace the two-body wave operators by the channel wave operators

$$\begin{aligned}
S_{\alpha\beta} &= \Omega_{\alpha+}^\dagger(H_0 + V_s, \Phi_\alpha, H_\alpha)\Omega_{\beta-}(H_0 + V_s, \Phi_\beta, H_\beta) \\
&\quad - i2\pi\delta(E_f - E_i)\Omega_{\alpha+}^\dagger(H_0 + V_s, \Phi_\alpha, H_\alpha)V_W\Omega_{\beta-}(H_0 + V_s, \Phi_\beta, H_\beta) \\
&\quad - 2\pi i\delta(E_f - E_i) \times \\
&\quad \Omega_{\alpha+}^\dagger(H_0 + V_s, \Phi_\alpha, H_\alpha)V_W \frac{1}{E_i - H_0 - V_s + i\epsilon} V_W\Omega_{\beta-}(H_0 + V_s, \Phi_\beta, H_\beta) + \dots
\end{aligned} \tag{154a}$$

$$\tag{154b}$$

$$\tag{154c}$$

$$\tag{154d}$$

Unitarity

The assumption that the range of Ω_\pm is the orthogonal complement of the subspace spanned by the bound states of H means that the scattering operator is unitary. This condition is called **asymptotic completeness**. It can be proved for some interactions, but it is normally assumed.

The scattering operator conserves energy so it can be represented

$$\langle E', \dots | S | E, \dots \rangle = \delta(E' - E) S(E)$$

Unitarity requires

$$S^\dagger S = I$$

which in the energy basis has the form

$$\langle E', \dots | S^\dagger S | E, \dots \rangle = \delta(E' - E) S(E) S^\dagger(E)$$

To be specific consider two body scattering in the CM frame. Normally the basis $|\hat{\mathbf{k}}, \mu_1 \mu_2\rangle$. To treat unitarity it is useful to transform to an energy basis

$$I = \int |k\rangle k^2 dk k = \int |k\rangle k^2 \frac{dk}{dE} dE k \int |k\rangle k^2 \frac{dk}{dE} dE k = \int |E\rangle dE E$$

which means

$$|k\rangle k \sqrt{\frac{dk}{dE}} = |E\rangle$$

for

$$E = \frac{k^2}{2\mu} \quad \frac{dk}{dE} = \frac{\mu}{k}$$

$$|k\rangle \sqrt{k\mu} = |E\rangle$$

$$\langle E, \hat{\mathbf{k}}, \nu_1 \nu_2 | S | E', \hat{\mathbf{k}}', \nu'_1, \nu'_2 \rangle$$

$$\delta(E-E') \delta(\hat{\mathbf{k}}-\hat{\mathbf{k}}') \delta_{\nu_1 \nu'_1} \delta_{\nu_2 \nu'_2} - 2\pi i \delta(E-E') \frac{1}{\sqrt{k\mu}} \langle E, \hat{\mathbf{k}}, \nu_1, \nu_2 | T(E+i\epsilon) | E', \hat{\mathbf{k}}', \nu'_1, \nu'_2 \rangle \frac{1}{\sqrt{k'\mu}}$$

$$|S(E) = I - 2\pi i T(E+i\epsilon)$$

Note that while the operator $T(E+i\epsilon)$ is function of $z = E+i\epsilon$, the operator does on commute with H . The unitarity condition becomes

$$I = I - 2\pi i (T(E+i\epsilon-) - T(E-i\epsilon)) + 4\pi^2 T^\dagger(E-i\epsilon) |E''\rangle dE'' \langle E | T(E+i\epsilon)$$

Summary of formulas:

Scattering probability

$$P = |\langle \Psi^+(0) | \Psi^-(0) \rangle|^2 = |\langle \Psi^+(t) | \Psi^-(t) \rangle|^2 \quad (155)$$

Scattering asymptotic condition initial conditions for scattering solutions

$$\lim_{t \rightarrow \pm\infty} \|\Psi^\pm(t) - \Psi_0^\pm(t)\| = 0 \quad (156)$$

Equations of motion interacting and non-interacting scattering solutions

$$i\hbar \frac{d|\Psi^\pm(t)\rangle}{dt} = H |\Psi^\pm(t)\rangle \quad (157)$$

$$i\hbar \frac{d|\Psi_0^\pm(t)\rangle}{dt} = H_0 |\Psi_0^\pm(t)\rangle \quad (158)$$

Møller wave operators
transform non-interacting to interacting scattering solutions

$$\Omega_{\pm} = \lim_{t \rightarrow \pm\infty} e^{iHt/\hbar} e^{-iH_0 t/\hbar} \quad (159)$$

$$|\Psi^{\pm}(t)\rangle = \Omega_{\pm} |\Psi_0^{\pm}(t)\rangle \quad (160)$$

Intertwining relation
leads to energy conservation in S

$$H\Omega_{\pm} = \Omega_{\pm}H_0 \quad (161)$$

Scattering operator
replace dependence on interacting wave packets by dependence on
non-interacting wave packets

$$P = |\langle \Psi_0^+(0) | \Omega_+^{\dagger} \Omega_- | \Psi_0^-(0) \rangle|^2 \quad (162)$$

$$P = |\langle \Psi_0^+(0) | S | \Psi_0^-(0) \rangle|^2 \quad (163)$$

$$S = \Omega_+^{\dagger} \Omega_- \quad (164)$$

$$[S, H_0] = 0 \quad (165)$$

Relation of S to dynamics

$$\langle \Psi_0^+(0) | S | \Psi_0^-(0) \rangle = \langle \Psi_0^+(0) | (I - 2\pi i \delta(E_+ - E_-) T(E_- + i\epsilon) | \Psi_0^-(0) \rangle \quad (166)$$

Transition operator

$$T(z) = V + V(z - H)^{-1}V \quad (167)$$

Lippmann Schwinger equation for the transition operator

$$T(z) = V + V(z - H_0)^{-1}T(z) \quad (168)$$

Solved form of scattering wave functions
Lippmann Schwinger equation for the scattering wave function

$$|\Psi^\pm(0)\rangle = |\mathbf{k}^\pm\rangle d\mathbf{k}\langle\mathbf{k}||\Psi_0^\pm(0)\rangle \quad (169)$$

$$\begin{aligned} |\mathbf{k}^\pm\rangle &= |\mathbf{k}\rangle + (\mathbf{k}^2/2\mu - H \mp i\epsilon)^{-1} V|\mathbf{k}\rangle = \\ &= |\mathbf{k}\rangle + (\mathbf{k}^2/2\mu - H_0 \mp i\epsilon)^{-1} V|\mathbf{k}^\pm\rangle \end{aligned} \quad (170)$$

Relation between scattering wave functions and transition operators

$$\langle\mathbf{k}'|T(\mathbf{k}^2/2\mu \pm i\epsilon)|\mathbf{k}\rangle = \langle\mathbf{k}'|V|\mathbf{k}^\mp\rangle \quad (171)$$

$$\langle\mathbf{k}'|T(\mathbf{k}'^2/2\mu \pm i\epsilon)|\mathbf{k}\rangle = \langle\mathbf{k}'^\pm|V|\mathbf{k}\rangle \quad (172)$$

Coordinate space representation of Lippmann Schwinger equation

$$\langle\mathbf{r}|\mathbf{k}^\pm\rangle = \langle\mathbf{r}|\mathbf{k}^\pm\rangle - \frac{\mu}{2\pi\hbar^2} \int \frac{e^{\mp ik|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') d\mathbf{r}' \langle\mathbf{r}'|\mathbf{k}\rangle \quad (173)$$

**Large r limit of scattering wave functions
scattering amplitude**

$$\lim_{r \rightarrow \infty} \langle\mathbf{r}|\mathbf{k}^\pm\rangle \rightarrow \frac{1}{(2\pi\hbar)^{3/2}} (e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} + \frac{e^{ikr}}{r} F(k\hat{\mathbf{r}}, \mathbf{k})) \quad (174)$$

Relation of transition operator to scattering amplitude

$$F(\mathbf{k}', \mathbf{k}) = -(2\pi)^2 \hbar \mu \langle\mathbf{k}|T(E + i\epsilon)|\mathbf{k}\rangle \quad (175)$$

Differential cross section

**removes dependence on free wave packets assuming that they are
narrow**

$$d\sigma = \frac{(2\pi)^4 \hbar^2}{v} |\langle\mathbf{p}'_1, \mathbf{p}'_2|T(E + i\epsilon)|\mathbf{p}_1, \mathbf{p}_2\rangle|^2 \delta(E' - E) \delta(\mathbf{P}' - \mathbf{P}) d\mathbf{p}'_1 d\mathbf{p}'_2 \quad (176)$$

**Exact form for transition rates
exact form of golden rule**

$$\begin{aligned} \frac{dP}{dt} &= \frac{2\pi}{\hbar} |\langle\mathbf{p}'_1, \mathbf{p}'_2|T(E + i\epsilon)|\mathbf{p}_1, \mathbf{p}_2\rangle|^2 \delta(E' - E) \delta(\mathbf{P}' - \mathbf{P}) d\mathbf{p}'_1 d\mathbf{p}'_2 = \\ &= \frac{2\pi}{\hbar} |\langle(\mathbf{p}'_1, \mathbf{p}'_2)^+|V_d|\mathbf{p}_1, \mathbf{p}_2\rangle|^2 \delta(E' - E) \delta(\mathbf{P}' - \mathbf{P}) d\mathbf{p}'_1 d\mathbf{p}'_2 \end{aligned} \quad (177)$$

Scattering phase shifts

$$S = e^{2i\delta} \quad (178)$$

Partial wave representation of phase shifts

$$\langle \mathbf{k}' | S | \mathbf{k} \rangle = \langle \mathbf{k}' | e^{2i\delta} | \mathbf{k} \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_m^l(\hat{\mathbf{k}}') e^{2i\delta_l(k)} Y_m^{l*}(\hat{\mathbf{k}}) \quad (179)$$

Two potential formulation of Gell Mann Low used in strong + Coulomb resonance calculations

$$H = H_0 + V_1 + V_2 \quad V_1 \gg V_2 \quad (180)$$

$$T(z) \approx T_1(z) + \Omega_{1+}^\dagger V_2 \Omega_{1-} \quad (181)$$

Impossibility of constructing V from S .

$$\lim_{t \rightarrow \pm\infty} \|(A - I)e^{-iH_0 t/\hbar} |\Psi\rangle\| = 0 \quad A^\dagger A = I \quad (182)$$

$$H' = A^\dagger H A = H_0 + V' \Leftrightarrow S' = S \quad (183)$$

Treatment of resonant decay

$$t_l \approx -\frac{1}{\pi\mu k} \frac{\Gamma/2}{E - E_b - \Delta E + i\Gamma/2} \quad (184)$$

$$\tau = \hbar/\Gamma \quad (185)$$

$$\Gamma = 2\pi \int \langle B | V_2 | \mathbf{k}' \rangle d\mathbf{k}' \delta(\mathbf{k}'^2/2\mu - \mathbf{k}^2/2\mu) \langle \mathbf{k}' | V_1 | B_1 \rangle \quad (186)$$

Optical theorem

construct total cross section from forward scattering amplitude

$$S^\dagger S = I \quad (187)$$

$$Im(F(\mathbf{k}, \mathbf{k})) = \frac{k}{4\pi\hbar} \sigma_t \quad (188)$$

$$\langle \mathbf{r} | \mathbf{k}^\pm \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_m^l(\hat{\mathbf{r}}) \langle r | k^\pm, l \rangle Y_m^{l*}(\hat{\mathbf{k}}) \quad (189)$$

Partial wave Lippmann Schwinger equation

$$\begin{aligned} \langle r|k^-, l\rangle = \\ \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}} (j_l(kr/\hbar) - i\frac{2\mu k}{\hbar^3} \int_0^\infty j_l(kr'</\hbar)h_l^1(kr'>/\hbar)r'^2 dr' V(r') \langle r|k^-, l\rangle \end{aligned} \quad (190)$$

Relation to partial wave transition operator

$$t_l(k, k, \mathbf{k}^2/2\mu + i\epsilon) = \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}} \int_0^\infty j_l(kr/\hbar)r'^2 dr' V(r') \langle r|k^\pm, l\rangle \quad (191)$$

Relation to phase shifts

$$f_l(k) = -(2\pi)^2 \mu \hbar t_l(k, k, \mathbf{k}^2/2\mu + i\epsilon) = \frac{4\pi\hbar}{k} e^{i\delta_l} \sin(\delta_l) \quad (192)$$

$$t_l(k, k, \mathbf{k}^2/2\mu + i\epsilon) = -\frac{1}{\pi\mu k} e^{i\delta_l} \sin(\delta_l) \quad (193)$$

$$\langle r|k^\pm, l\rangle \rightarrow \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}} \frac{\hbar}{kr} e^{i\delta_l} \sin(\delta_l) \quad (194)$$

Identical particles

$$F(\mathbf{k}', \mathbf{k}) \rightarrow (F(\mathbf{k}', \mathbf{k}) \pm F(-\mathbf{k}', \mathbf{k})) \quad (195)$$

$$F(k, \theta) \rightarrow (F(k, \theta) \pm F(k, \pi - \theta)) \quad (196)$$