Scattering Theory

In quantum mechanics the basic observable is the probability

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

for a transition from and 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:

$$P(t) = |\langle \psi^+(t)|\psi^-(t)\rangle|^2 = |\langle \psi^+(0)|e^{iHt/\hbar}e^{-iHt/\hbar}\psi^-(0)\rangle|^2 =$$

$$|\langle \psi^+(0)|\psi^-(0)\rangle|^2 = P(0) \tag{2}$$

For a scattering experiment $|\psi^-(t)\rangle$ represents the state of the beam and target. It is a solution of the Schrödinger equation that looks like a free beam of particles heading towards 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 associated with the photomultiplier tubes.

The scattering probability has to be evaluated at (any) 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 they look like free particles:

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

where

$$|\Psi_0^\pm(\pm T)\rangle \tag{4}$$

are the corresponding free particle solutions at $t = -T$ and $t = T$. The free particle solutions satisfy the free-particle Schrödinger equation:

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

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

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

$$|\Psi_0^\pm(t)\rangle = U_0(t \mp T)|\Psi^\pm(T)\rangle \qquad U_0(t) = e^{-iH_0t/\hbar} \tag{7}$$

The initial free particle wave packets can be taken as minimal uncertainty wave packets with momentum uncertainty Δp_1 and Δp_2 and specified mean single-particle momenta, $\mathbf{p}_{10}$ and $\mathbf{p}_{20}$. These states have the form

$$\langle \mathbf{p}_1, \mathbf{p}_2 | \Psi_0^{\pm}(t) \rangle =$$

$$\frac{1}{(2\pi)^{3/4}} \frac{1}{(\Delta p_1)^{3/2}} e^{-\frac{(\mathbf{p}_1 - \mathbf{p}_{10})^2}{(2\Delta p_1)^2}} \frac{1}{(2\pi)^{3/4}} \frac{1}{(\Delta p_1)^{3/2}} e^{-\frac{(\mathbf{p}_2 - \mathbf{p}_{20})^2}{(2\Delta p_2)^2}} e^{-i(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2})t/\hbar}. \quad (8)$$

Of course in a real experiment we do not have 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 measured in an experiment is counts in the photo-multiplier tubes. It is also awkward to determine the times $\pm T$. 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 below.

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 $U(t) = e^{-iHt/\hbar} \to U_0(t) = e^{-iH_0 t/\hbar}$. This means that if

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

then

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

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 $T \to \infty$, which does not change the initial condition for short range V. This leads to the **scattering asymptotic conditions**:

$$0 = \lim_{t\to\pm\infty} \| |\Psi^{\pm}(t)\rangle - |\Psi_0^{\pm}(t)\rangle \| =$$

$$\lim_{t\to\pm\infty} \| e^{-iH\frac{t}{\hbar}} |\Psi^{\pm}(0)\rangle - e^{-iH_0\frac{t}{\hbar}} |\Psi_0^{\pm}(0)\rangle \| =$$

$$\lim_{t\to\pm\infty} \| |\Psi^{\pm}(0)\rangle - e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}} |\Psi_0^{\pm}(0)\rangle \|. \quad (11)$$

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

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

The operators,

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

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

$$\Omega_\pm := I + \int_0^{\pm\infty} \frac{d}{dt} e^{iH\frac{t}{\hbar}} e^{-iH_0\frac{t}{\hbar}} dt =$$

$$I + \frac{i}{\hbar}\int_0^{\pm\infty} e^{iH\frac{t}{\hbar}} V e^{-iH_0\frac{t}{\hbar}} dt$$

Convergence follows provided

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

A sufficient condtion for this to be finite is

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

Wheather this is true depends on the choice of potential. It holds for most potentials that fall off faster than the Coulomb potential at ∞. In what follows we assume that the Møller wave operators exist.

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

$$H\Omega_\pm = \Omega_\pm H_0. \tag{14}$$

To prove (14) note that

$$e^{iH\frac{s}{\hbar}}\Omega_\pm = \lim_{(t+s)\to\pm\infty} e^{iH\frac{(t+s)}{\hbar}} e^{-iH_0\frac{(t+s)}{\hbar}} e^{iH_0\frac{s}{\hbar}} = \Omega_\pm e^{iH_0\frac{s}{\hbar}}. \tag{15}$$

Differentiation with respect to s, setting s to zero gives (14). This condition ensure that energy is conserved in the scattering experiment; i.e. that

$$H\Omega_\pm|E_0\rangle = \Omega_\pm H_0|E_0\rangle = E_0\Omega_\pm|E_0\rangle \tag{16}$$

which show that $\Omega_\pm$ maps eigenstates of H_0 with energy E_0 to eignestates of H with the same energy.

It also follows that

$$|\Psi^\pm(t)\rangle = U(t)|\Psi^\pm(0)\rangle =$$

$$U(t)\Omega_\pm|\Psi_0^\pm(0)\rangle = \Omega_\pm U_0(t)|\Psi_0^\pm(0)\rangle = \Omega_\pm|\Psi_0^\pm(t)\rangle \tag{17}$$

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

$$P = |\langle\Psi_0^+(t)|\Omega_+^\dagger\Omega_-|\Psi_0^-(t)\rangle|^2 \tag{18}$$

which is independent of t by (17).

The **scattering operator** S operator is defined by

$$S := \Omega_+^\dagger \Omega_- . \tag{19}$$

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

$$P = |\langle \Psi_0^+(t)|S|\Psi_0^-(t)\rangle|^2 . \tag{20}$$

The advantage of expressing the probability in terms of the the free-particle states is that they have a simple form that is determined by the measurement, but 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 plane-wave matrix elements of the scattering operator

$$\langle \Psi_0^+|S|\Psi_0^-\rangle =$$

$$\int \langle \Psi_0^+|\mathbf{p}_1, \mathbf{p_2}\rangle d\mathbf{p}_1 d\mathbf{p}_2 \langle \mathbf{p}_1, \mathbf{p_2}|S|\mathbf{p}_1', \mathbf{p_2}'\rangle d\mathbf{p}_1' d\mathbf{p}_2' \langle \mathbf{p}_1', \mathbf{p_2}'|\Psi_0^-\rangle . \tag{21}$$

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

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \tag{22}$$

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

$$\mathbf{k} := \mathbf{p}_1 - \frac{m_1}{m_1 + m_2}\mathbf{P} = \frac{m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2}{m_1 + m_2}, \tag{23}$$

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

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

The Jacobian of the variable change

$$(\mathbf{p}_1, \mathbf{p}_2) \to (\mathbf{P}, \mathbf{k}) \tag{25}$$

is 1.

In terms of these variables the scattering probability amplitude can be expressed as

$$\int \langle \Psi_0^+|\mathbf{k}, \mathbf{P}\rangle d\mathbf{k} d\mathbf{P} \langle \mathbf{k}, \mathbf{P}|S|\mathbf{k}', \mathbf{P}'\rangle d\mathbf{k}' d\mathbf{P}' \langle \mathbf{k}', \mathbf{P}'|\Psi_0^-\rangle \tag{26}$$

The kernel of this expression has the form

$$\langle \mathbf{k}, \mathbf{P}|S|\mathbf{k}', \mathbf{P}'\rangle =$$
$$\lim_{t\to\infty} \langle \mathbf{k}, \mathbf{P}|e^{iH_0 t/\hbar} e^{-2iHt/\hbar} e^{iH_0 t/\hbar}|\mathbf{k}', \mathbf{P}'\rangle =$$
$$\delta(\mathbf{P}-\mathbf{P}')\delta(\mathbf{k}-\mathbf{k}') + \int_0^\infty \frac{d}{dt}\langle \mathbf{k}, \mathbf{P}|e^{iH_0 t/\hbar} e^{-2iHt/\hbar} e^{iH_0 t/\hbar}|\mathbf{k}', \mathbf{P}'\rangle =$$
$$\delta(\mathbf{P}-\mathbf{P}')\delta(\mathbf{k}-\mathbf{k}') - \frac{i}{\hbar}\int_0^\infty \langle \mathbf{k}, \mathbf{P}|e^{iH_0 t/\hbar} V e^{-2iHt/\hbar} e^{iH_0 t/\hbar}|\mathbf{k}', \mathbf{P}'\rangle -$$
$$\frac{i}{\hbar}\int_0^\infty \langle \mathbf{k}, \mathbf{P}|e^{iH_0 t/\hbar} e^{-2iHt/\hbar} V e^{iH_0 t/\hbar}|\mathbf{k}', \mathbf{P}'\rangle \tag{27}$$

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

$$H = \frac{\mathbf{P}^2}{2M} + h \qquad h = \frac{\mathbf{k}^2}{2\mu} + V \tag{28}$$

$$H_0 = \frac{\mathbf{P}^2}{2M} + h_0 \qquad h_0 = \frac{\mathbf{k}^2}{2\mu}. \tag{29}$$

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

$$e^{iHt/\hbar} e^{-iH_0 t/\hbar} = e^{iht/\hbar} e^{-ih_0 t/\hbar}. \tag{30}$$

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

$$\langle \mathbf{P}, \mathbf{k}|O|\mathbf{P}', \mathbf{k}'\rangle =: \delta(\mathbf{P}-\mathbf{P}')\langle \mathbf{k}|\hat{O}|\mathbf{k}'\rangle \tag{31}$$

Thus, assuming a translationally invariant interaction, (27) becomes

$$\delta(\mathbf{P}-\mathbf{P}')\Bigg(\delta(\mathbf{k}-\mathbf{k}') - \frac{i}{\hbar}\int_0^\infty \langle \mathbf{k}|e^{ih_0 t/\hbar}\hat{V} e^{-2iht/\hbar} e^{ih_0 t/\hbar}|\mathbf{k}'\rangle -$$
$$\frac{i}{\hbar}\int_0^\infty \langle \mathbf{k}|e^{ih_0 t/\hbar} e^{-2iht/\hbar}\hat{V} e^{ih_0 t/\hbar}|\mathbf{k}'\rangle\Bigg) \tag{32}$$

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

$$h_0|\mathbf{k}\rangle = \frac{\mathbf{k}^2}{2\mu}|\mathbf{k}\rangle = E(k)|\mathbf{k}\rangle. \tag{33}$$

I define the average relative kinetic energy

$$\bar{E} = \frac{1}{2}(E(k) + E(k')). \tag{34}$$

Using (33) and (34) in (32) gives

$$\delta(\mathbf{P}-\mathbf{P}')\left(\delta(\mathbf{k}-\mathbf{k}')-\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|e^{ih_0t/\hbar}\hat{V}e^{-2iht/\hbar}e^{ih_0t/\hbar}|\mathbf{k}'\rangle-\right.$$
$$\left.\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|e^{ih_0t/\hbar}e^{-2iht/\hbar}\hat{V}e^{ih_0t/\hbar}|\mathbf{k}'\rangle\right)=$$
$$\delta(\mathbf{P}-\mathbf{P}')\left(\delta(\mathbf{k}-\mathbf{k}')-\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|\hat{V}e^{-2i(h-\bar{E})t/\hbar}|\mathbf{k}'\rangle-\right.$$
$$\left.\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|e^{-2i(h-\bar{E})t/\hbar}\hat{V}|\mathbf{k}'\rangle\right)\tag{35}$$

These limits only make sense if they are used in (27) where the integrals over $\mathbf{k}, \mathbf{P}$ and $\mathbf{k}'$ are performed *before* the time integrals. After such an integration the result will vanish for large t. This can be seen by considering the example

$$\int f(k)e^{\frac{-ik^2t}{2\mu\hbar}}d^3k=\int\hat{f}(k^2)e^{\frac{-ik^2t}{2\mu\hbar}}k^2dk=$$
$$(\frac{2\mu\hbar}{t})^{3/2}\int\hat{f}(\frac{2\mu\hbar}{t}u^2)e^{-iu^2}u^2du\tag{36}$$

where

$$\hat{f}(k^2):=\int f(\mathbf{k})d\hat{\mathbf{k}}\tag{37}$$

This falls off like $t^{-3/2}$ for large t. It we insert an additional factor $e^{-\epsilon t}$ which 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 integral in the limit that $\epsilon\to 0$. On the other hand if we insert this factors the order of integration does not matter, and we can perform the time integral first, with the understanging that $\lim_{\epsilon\to 0}$ be taken after integrating over the initial and final wave packets. It follows that (35) can be replaced by

$$\delta(\mathbf{P}-\mathbf{P}')\left(\delta(\mathbf{k}-\mathbf{k}')-\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|\hat{V}e^{-2i(h-\bar{E}-i\epsilon)t/\hbar}|\mathbf{k}'\rangle-\right.$$
$$\left.\frac{i}{\hbar}\int_0^\infty\langle\mathbf{k}|e^{-2i(h-\bar{E}i-i\epsilon)t/\hbar}\hat{V}|\mathbf{k}'\rangle\right)\tag{38}$$

Doing the time integral gives

$$\delta(\mathbf{P}-\mathbf{P}')\left(\delta(\mathbf{k}-\mathbf{k}')+\frac{1}{2}\langle\mathbf{k}|\hat{V}\frac{1}{\bar{E}-h+i\epsilon}|\mathbf{k}'\rangle+\right.$$
$$\left.+\frac{1}{2}\langle\mathbf{k}|\frac{1}{\bar{E}-h+i\epsilon}\hat{V}|\mathbf{k}'\rangle\right)\tag{39}$$

Some care is required to evaluate (39). The second resolvent identities

$$\frac{1}{z-A} - \frac{1}{z-B} = \frac{1}{z-A}(A-B)\frac{1}{z-B} = \frac{1}{z-B}(A-B)\frac{1}{z-A} \tag{40}$$

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

$$\frac{1}{\bar{E}-h+i\epsilon} - \frac{1}{\bar{E}-h_0+i\epsilon} =$$
$$\frac{1}{\bar{E}-h_0+i\epsilon} V \frac{1}{\bar{E}-h+i\epsilon} =$$
$$\frac{1}{\bar{E}-h+i\epsilon} V \frac{1}{\bar{E}-h_0+i\epsilon} \tag{41}$$

Using these in (39) gives

$$\delta(\mathbf{P}-\mathbf{P}') \Big(\delta(\mathbf{k}-\mathbf{k}') + \frac{1}{2}\langle \mathbf{k}|\hat{V}(1+\frac{1}{\bar{E}-h+i\epsilon}\hat{V})\frac{1}{\bar{E}-h_0+i\epsilon}|\mathbf{k}'\rangle +$$
$$+\frac{1}{2}\langle \mathbf{k}|\frac{1}{\bar{E}-h_0+i\epsilon}(1+\hat{V}\frac{1}{\bar{E}-h+i\epsilon}\hat{V})|\mathbf{k}'\rangle \Big) =$$
$$\delta(\mathbf{P}-\mathbf{P}') \Big(\delta(\mathbf{k}-\mathbf{k}') + \frac{1}{2}\langle \mathbf{k}|(\hat{V}+\hat{V}\frac{1}{\bar{E}-h+i\epsilon}\hat{V})|\mathbf{k}'\rangle(\frac{1}{\bar{E}-E(k')+i\epsilon} + \frac{1}{\bar{E}-E(k)+i\epsilon}) \Big)$$
$$\delta(\mathbf{P}-\mathbf{P}') \Big(\delta(\mathbf{k}-\mathbf{k}') + \frac{1}{2}\langle \mathbf{k}|(\hat{V}+\hat{V}\frac{1}{\bar{E}-h+i\epsilon}\hat{V})|\mathbf{k}'\rangle(\frac{1}{\bar{E}-E(k')+i\epsilon} + \frac{1}{\bar{E}-E(k)+i\epsilon}) \Big) =$$
$$\delta(\mathbf{P}-\mathbf{P}') \Big(\delta(\mathbf{k}-\mathbf{k}') - \langle \mathbf{k}|(\hat{V}+\hat{V}\frac{1}{\bar{E}-h+i\epsilon}\hat{V})|\mathbf{k}'\rangle \frac{2i\epsilon}{(E(k')-E(k))^2+\epsilon^2} \Big) \tag{42}$$

In the limit that $\epsilon \to 0$

$$\frac{2i\epsilon}{(E(k')-E(k))^2+\epsilon^2} \to -2\pi i \delta(E(k')-E(k)) \tag{43}$$

which implies that (39) becomes

$$\langle \mathbf{P},\mathbf{k}|S|\mathbf{P}',\mathbf{k}'\rangle =$$
$$\delta(\mathbf{P}-\mathbf{P}') \Big(\delta(\mathbf{k}-\mathbf{k}') - 2\pi i \delta(E(k)-E(k'))\langle \mathbf{k}|(\hat{T}(E-h+i\epsilon)|\mathbf{k}'\rangle \Big) \tag{44}$$

Where operator

$$\hat{T}(z) := \hat{V} + \hat{V}\frac{1}{z-h}\hat{V} \tag{45}$$

is called the the **transition operator**. Using the second resolvent identities (41) in (45) shows that $\hat{T}(z)$ satisfies the integral equation

$$\hat{T}(z) := \hat{V} + \hat{V}\frac{1}{z-h_0}\hat{T}(z) \tag{46}$$

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

These are called **Lippmann-Schwinger equations** for the transition operator. We are normally interested in the case $z = E + i\epsilon = \frac{\mathbf{k}^2}{2\mu} + i\epsilon$.

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

$$\langle\Psi^+|\Psi^-\rangle = \langle\Psi_0^+|S|\Psi_0^-\rangle =$$
$$\int \langle\Psi_0^+|\mathbf{k},\mathbf{P}\rangle d\mathbf{k}d\mathbf{P}\langle\mathbf{k},\mathbf{P}|S|\mathbf{k}',\mathbf{P}'\rangle d\mathbf{k}'d\mathbf{P}'\langle\mathbf{k}',\mathbf{P}'|\Psi_0^-\rangle \tag{48}$$

with

$$\langle\mathbf{k},\mathbf{P}|S|\mathbf{k}'\mathbf{P}'\rangle =$$
$$\delta(\mathbf{P}-\mathbf{P}')\Big(\delta(\mathbf{k}-\mathbf{k}') - 2\pi i\delta(E(k)-E(k'))\langle\mathbf{k}|\hat{T}(E+i\epsilon)|\mathbf{k}'\rangle\Big) \tag{49}$$

and

$$\hat{T}(E+i\epsilon) = \hat{V} + \hat{V}\frac{1}{E - h_0 + i\epsilon}\hat{T}(E+i\epsilon) \tag{50}$$

Calculation of the scattering operator using the interaction picture:

The scattering operator can be expressed as

$$S := \Omega_+^\dagger\Omega_- = \lim_{t\to\infty,t'\to-\infty} e^{iH_0\frac{t}{\hbar}}e^{-iH\frac{(t-t')}{\hbar}}e^{-iH_0\frac{t'}{\hbar}} = \lim_{t\to\infty,t'\to-\infty} U_I(t,t') \tag{51}$$

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

$$i\hbar\frac{d}{dt}U_I(t,t') = V_I(t)U_I(t,t') \qquad U_I(t',t') = I \tag{52}$$

where

$$V_I(t) = e^{\frac{iH_0t}{\hbar}}Ve^{\frac{-iH_0t}{\hbar}} \tag{53}$$

is the interaction picture interaction. The formal solution can be obtained by iterating the integrated form of (52)

$$U(t,t') = I - \frac{i}{\hbar}\int_{t'}^{t} V_I(t'')U(t'',t')dt'' \tag{54}$$

The formal solution of this equation is

$$S = I + \sum_{n=0}^{\infty}(\frac{-i}{\hbar})^n\frac{1}{n!}\int_{-\infty}^{\infty} T(V_I(t_1)\cdots V_I(t_n))dt_1\cdots dt_n =:$$
$$T\exp(-\frac{i}{\hbar}\int_{-\infty}^{\infty} V_I(t')dt') \tag{55}$$

which is expressed as a time-ordered exponential. This is obtained by replacing the n-nested integrals by equivalent integrals obtained by the $n!$ possible orders of integration of the time integrals.

This method is used 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 $e^{2T\|V\|/\hbar}$.

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

$$P = |\langle \Psi_0^+(0)|S|\Phi_0^-(0)\rangle|^2. \tag{56}$$

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

$$e^{iHt/\hbar}e^{-iH_0t/\hbar} = e^{iht/\hbar}e^{-ih_0t/\hbar}. \tag{57}$$

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

$$\langle \mathbf{P}, \mathbf{k}|\Omega^\pm|\mathbf{P}', \mathbf{k}'\rangle = \delta(\mathbf{P} - \mathbf{P}')\langle \mathbf{k}|\hat{\Omega}^\pm|\mathbf{k}'\rangle \tag{58}$$

where

$$\hat{\Omega}^\pm = \lim_{t\to\pm\infty} e^{iht/\hbar}e^{-ih_0t/\hbar}. \tag{59}$$

The scattering eigenstates are defined as

$$|\mathbf{k}^\pm\rangle = \hat{\Omega}^\pm|\mathbf{k}\rangle. \tag{60}$$

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

$$h\hat{\Omega}_\pm = \hat{\Omega}_\pm h_0 \tag{61}$$

imply that these are eigenstates of h with energy $\frac{k^2}{2\mu}$:

$$h|\mathbf{k}^\pm\rangle = h\hat{\Omega}^\pm|\mathbf{k}\rangle\hat{\Omega}^\pm h_0|\mathbf{k}\rangle = \frac{k^2}{2\mu}\hat{\Omega}^\pm|\mathbf{k}\rangle = \frac{k^2}{2\mu}|\mathbf{k}^\pm\rangle. \tag{62}$$

These solutions are related to the S matrix by

$$P = |\langle \Psi^+(0)|\Psi^-(0)\rangle|^2 \tag{63}$$

where

$$\langle \mathbf{P}, \mathbf{k}|\Psi^{\pm}(0)\rangle = \int \langle \mathbf{k}|\mathbf{k}^{\pm\prime}\rangle d\mathbf{P} d\mathbf{k}' \langle \mathbf{P}, \mathbf{k}|\Psi_0^{\pm}(0)\rangle. \tag{64}$$

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

$$|\mathbf{k}^{\pm}\rangle := \lim_{t\to\pm\infty} e^{-iht/\hbar} e^{ih_0 t/\hbar}|\mathbf{k}\rangle =$$

$$(I + \lim_{t\to\pm\infty} \int_0^t \frac{d}{dt} e^{-iht/\hbar} e^{ih_0 t/\hbar}|\mathbf{k}\rangle). \tag{65}$$

If I include the wave packet (**??**) becomes

$$|\psi_0^{\pm}\rangle + \lim_{t\to\pm\infty} \int_0^t \frac{d}{dt} \int d\mathbf{k} e^{iht/\hbar} e^{-ih_0 t/\hbar}|\mathbf{k}\rangle \psi_0^{pm}(\mathbf{k}) \tag{66}$$

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

$$|\psi_0^{\pm}\rangle + \lim_{\epsilon\to 0} \int_0^{\pm\infty} e^{\mp\epsilon t} \frac{d}{dt} \int d\mathbf{k} (e^{iht/\hbar} e^{-ih_0 t/\hbar})|\mathbf{k}\rangle \psi_0^{pm}(\mathbf{k})). \tag{67}$$

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 buy performing the time integral first, with the understanding that the integral must eventually integrated against a wave packet.

It follows that the integral in (**??**) becomes

$$|\mathbf{k}^{\pm}\rangle =$$

$$|\mathbf{k}\rangle + \lim_{\epsilon\to 0} \int_0^{\pm\infty} e^{\mp\epsilon t} \frac{d}{dt} (e^{iht/\hbar} e^{-ih_0 t/\hbar})|\mathbf{k}\rangle dt =$$

$$|\mathbf{k}\rangle - \lim_{\epsilon\to 0} (\frac{i}{\hbar}) \int_0^{\pm\infty} e^{\mp\epsilon t} e^{iht/\hbar} \hat{V} e^{-ih_0 t/\hbar}|\mathbf{k}\rangle dt =$$

$$|\mathbf{k}\rangle - \lim_{\epsilon\to 0} (\frac{i}{\hbar}) \int_0^{\pm\infty} e^{i(h-E(k)\pm i\epsilon)t/\hbar} \hat{V}|\mathbf{k}\rangle dt =$$

$$|\mathbf{k}\rangle + \lim_{\epsilon\to 0} \frac{1}{E(k) - h \mp i\epsilon} \hat{V}|\mathbf{k}\rangle \tag{68}$$

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

This gives the following expression for the scattering eigenstates

$$|\mathbf{k}^{\pm}\rangle = (I + \frac{1}{E(k) - h \pm i\epsilon} \hat{V})|\mathbf{k}\rangle \tag{69}$$

The operator

$$\frac{1}{z-h} \tag{70}$$

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

$$\frac{1}{z-h} - \frac{1}{z-h_0} = \frac{1}{z-h_0} V \frac{1}{z-h} = \frac{1}{z-h} V \frac{1}{z-h_0}. \tag{71}$$

Using these in the above expression with $z = E(k) \pm i\epsilon$ gives

$$|\mathbf{k}^\pm\rangle =$$

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

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

$$|\mathbf{k}\rangle + \frac{1}{E(k) - h_0 \pm i\epsilon}\hat{V}|\mathbf{k}^\pm\rangle \tag{72}$$

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

$$|\mathbf{k}^\pm\rangle = |\mathbf{k}\rangle + (\frac{\mathbf{k}^2}{2\mu} \mp i\epsilon^+ - h_0)^{-1}\hat{V}|\mathbf{k}^\pm\rangle. \tag{73}$$

This equation can be expressed in any basis

$$\langle\mathbf{r}|\mathbf{k}^\pm\rangle = \langle\mathbf{r}|\mathbf{k}\rangle + \int \langle\mathbf{r}|(\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{H}_0)^{-1}|\mathbf{r}'\rangle d\mathbf{r}'\hat{V}(\mathbf{r}')\langle\mathbf{r}|\mathbf{k}^\pm\rangle, \tag{74}$$

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

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

$$\langle\mathbf{r}|(\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{H}_0)^{-1}|\mathbf{r}'\rangle = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{k}\frac{2\mu e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')/\hbar}}{\mathbf{k}^2 - \mathbf{k}' \mp \epsilon} =$$

$$-\frac{\mu}{2\pi\hbar^2}\frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|} \tag{76}$$

Multiplying (72) by V and comparing to (45) gives

$$V|\mathbf{k}^\pm\rangle = V|\mathbf{k}\rangle + V\frac{1}{E(k) - h_0 \mp i\epsilon}V|\mathbf{k}\rangle = T(E \mp i\epsilon)|\mathbf{k}\rangle \tag{77}$$

It follows that the scattered wave functions can be expressed in terms of the **transition operator**, $T(z)$:

$$|\mathbf{k}^\pm\rangle = |\mathbf{k}\rangle + (\frac{\mathbf{k}^2}{2\mu} \mp i0^+ - \hat{h}_0)^{-1}\hat{T}(\frac{\mathbf{k}^2}{2\mu} \mp i0^+)|\mathbf{k}\rangle \tag{78}$$

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

$$\langle \mathbf{k}^{+\prime} | \hat{V} | \mathbf{k} \rangle = \langle \mathbf{k}' | \hat{V} | \mathbf{k}^- \rangle = \langle \mathbf{k}' | \hat{T}(\frac{\mathbf{k}^2}{2\mu} + i0^+) | \mathbf{k} \rangle \tag{79}$$

any of these can be used to calculate

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

$$\delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k} | (\hat{T}(E - h + i\epsilon) | \mathbf{k}' \rangle \right) =$$

$$\delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k} | (\hat{V} | \mathbf{k}^{-\prime} \rangle \right) =$$

$$\delta(\mathbf{P} - \mathbf{P}') \left(\delta(\mathbf{k} - \mathbf{k}') - 2\pi i \delta(E(k) - E(k')) \langle \mathbf{k}^+ | (\hat{V} | \mathbf{k}' \rangle \right) \tag{80}$$

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 in the Lippmann-Schwinger equations and then truncating the sum to a finite number (M) of terms

$$\langle n | \hat{T}(z) \approx \langle n | \hat{V} + \sum_m^M \langle n | \hat{V} (z - \hat{H}_0)^{-1} | m \rangle \langle m | \hat{T}(z) \tag{81}$$

Mathematically the justification for this procedure follows because the kernel of this equation is a compact operator (on a normed space which may or may not be the Hilbert space). Compactness means that it can be uniformly approximated by a finite rank matrix. Eq. (81) 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 approximations to $T(z)$:

$$\hat{T}(z) \approx \hat{V} + \sum_m \hat{V} (z - \hat{H}_0)^{-1} | m \rangle \langle m | \hat{T}(z) \tag{82}$$

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

Scattering cross sections

The notion of a scattering cross section is introduced to eliminate the dependence on the choice of wave packet in describing a scattering experiment.

In a real experiment there is a beam of particles moving with some mean momentum descirbed by an ensemble represented by a denstiy matrix

$$\rho_b = \sum_n P_{bn} | \phi_{bn} \rangle \langle \phi_{bn} |.$$

These particles directed at a target that is also an ensemble of target particles represented by another density matrix:

$$\rho_t = \sum_m P_{tm}|\phi_{tm}\rangle\langle\phi_{tm}|.$$

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.

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.

The starting point is to observe that 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 state $|\Psi\rangle$ is

$$dP = |\langle \mathbf{p}_1, \mathbf{p}_2|\Psi\rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 \tag{83}$$

For the case of interest the initial states can be expressed in terms of the scattering operator and the asymptotic free particle beam and target distributions

$$\langle \mathbf{p}_1, \mathbf{p}_2|\Psi\rangle = \langle \mathbf{p}_1, \mathbf{p}_2|S|\Psi_0^-\rangle \tag{84}$$

which is the 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 $S \to I$, so that part if S that causes the scattering is $(S - I)$. Replacing S by $S - I$ in (84) and replacing the initial state by the beam and target density matrices gives

$$dP = |\langle \mathbf{p}_1, \mathbf{p}_2|(S - I)|\rho_b\rho_t(S - I)^\dagger|\mathbf{p}_1, \mathbf{p}_2\rangle d\mathbf{p}_1 d\mathbf{p}_2 =$$

$$\sum_{mn} |\langle \mathbf{p}_1, \mathbf{p}_2| - 2\pi i\delta(E_f - E_i)T(E + i0)|\phi_{bn}\phi_{tm}\rangle|^2 P_{bn}P_{tm} d\mathbf{p}_1 d\mathbf{p}_2 \tag{85}$$

Of interest 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 above becomes

$$dP = \sum_{mn} P_{bn}P_{tm}|\langle \mathbf{p}_1, \mathbf{p}_2| - 2\pi i\delta(E_f - E_i)\delta(\mathbf{P}_f - \mathbf{P}_i)\hat{T}(E + i0)|\phi_{bn}\phi_{tm}\rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2 =$$

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

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

Now we make the crucial approximation - we assume that wave functions in the initial beam and target ensemples are sharply peaked around fixed values $\mathbf{p}_b$ and $\mathbf{p}_t$ respectively. We also assume that T does not change significantly on the scales of momenta where the wave packets are non-zero. For sharply peaked wave functions the following

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

replaces

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

which leaves

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

Representing the delta functions in the integral by

$$\delta(E_i' - E_i'')\delta(\mathbf{P}_f'' - \mathbf{P}_i') =$$
$$\frac{1}{(2\pi\hbar)^4} e^{i(\mathbf{p}_1' + \mathbf{p}_2' - \mathbf{p}_1'' - \mathbf{p}_2'')\cdot\mathbf{x}/\hbar} e^{-i(E_1' + E_2' - E_1'' - E_2'')t/\hbar} \cdot \mathbf{x} \tag{90}$$

and observing

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

The expression for the differential probability becomes

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

The integral shows that the probability get contributions from all times when both the n^{th} beam and m^{th} target particles are at the same place. It follows that the probability of a transition per unit time pert unit volume into volumes $d\mathbf{p}_1$ and $d\mathbf{p}_2$ about $\mathbf{p}_1$ and $\mathbf{p}_2$ is

$$\frac{dP}{dVdt} = \sum_{mn} P_{bn} P_{tm} 4\pi^2 \int \delta(\frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} - \frac{\mathbf{p}_t^2}{2m_t} - \frac{\mathbf{p}_b^2}{2m_b})\delta(\mathbf{1}_1 + \mathbf{p}_2 - \mathbf{p}_t - \mathbf{p}_b)\times$$
$$|\langle \mathbf{p}_1, \mathbf{p}_2|\hat{T}(E+i0)|\mathbf{p}_t, \mathbf{p}_b\rangle|^2 d\mathbf{p}_1 d\mathbf{p}_2$$
$$\frac{(2\pi\hbar)^6}{(2\pi\hbar)^4}|\phi_{tm}(\mathbf{x},t)|^2|\phi_{bn}(\mathbf{x},t)|^2 \tag{93}$$

The quantities

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

represent the probability 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 by the total number of beam and target particles then third expression becomes the number of scattering events within $d\mathbf{x}$ of $\mathbf{x}$ at time t.

If the interactions are sufficiently weak that essentially each particle experiences at most one collision, then we expect this rate to be proportional to the target density and the number of beam particle crossing a surface per unit time. In this case

$$\frac{dN}{dVdt} = d\sigma \sum_m N_t P_{mt}\phi_{t0}(\mathbf{x},t)|^2 \sum_n N_b P_{bn}|\phi_{b0}(\mathbf{x},t)|^2 = N_t N_b \frac{dP}{dVdt} \tag{95}$$

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

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

In using this expression, because of the δ functions there are 2 independent parameters needed to define the final state, one picks out 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

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

The relative velocity of the beam and target is

$$\mathbf{v} = \frac{\mathbf{k}}{m_1} - \frac{-\mathbf{k}}{m_2} = \frac{\mathbf{k}}{\mu} \tag{98}$$

With these substitutions

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

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

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

where

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

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:

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

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

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

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

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

For large r this becomes

$$\langle\mathbf{r}|\mathbf{k}^-\rangle \to \langle\mathbf{r}|\mathbf{k}\rangle - \frac{\mu}{2\pi\hbar^2}\frac{e^{ikr}}{r}e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}d\mathbf{r}'\hat{V}(\mathbf{r}')\langle\mathbf{r}|\mathbf{k}^-\rangle =$$

$$\frac{1}{(2\pi\hbar)^{3/2}}(e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} - (2\pi\hbar)^3\frac{\mu}{2\pi\hbar^2}\frac{e^{\pm ikr}}{r}\frac{1}{(2\pi\hbar)^{3/2}}e^{\mu ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\langle\mathbf{r}'|\mathbf{k}^\pm\rangle =$$

$$\frac{1}{(2\pi\hbar)^{3/2}}(e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} - (2\pi)^2\hbar\mu\frac{e^{\pm ikr}}{r}\langle k\hat{\mathbf{r}}|\hat{T}(E+i\epsilon)|\mathbf{k}\rangle)$$

$$\frac{1}{(2\pi\hbar)^{3/2}}(e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} + \frac{e^{\pm ikr}}{r}F(k\hat{\mathbf{r}},\mathbf{k}))$$

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

$$S = e^{2i\delta} \tag{104}$$

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

$$\delta(E-E')e^{2i\delta(E)} = \delta(E-E')(\hat{I} - 2\pi i \langle E|\hat{T}(E+i\epsilon)|E\rangle) =$$

$$\delta(E-E')(\hat{I} - i\frac{2\pi\mu}{k}\langle k|\hat{T}(E+i\epsilon)|k\rangle) \tag{105}$$

This gives

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

or

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

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

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

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

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

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

The integral term is

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

$$\frac{(2\pi\hbar)^{3/2}}{4\pi}(-1\frac{1}{\pi k\mu}e^{i\delta_l}\sin(\delta_l) \tag{110}$$

Summary of formulas:

Scattering probability

$$P = |\langle\Psi^+(0)|\Psi^-(0)\rangle|^2 = |\langle\Psi^+(t)|\Psi^-(t)\rangle|^2 \tag{111}$$

Scattering asymptotic condition
initia conditions for scattering solutions

$$\lim_{t\to\pm\infty} \| |\Psi^{\pm}(t)\rangle - |\Psi_0^{\pm}(t)\rangle \| = 0 \tag{112}$$

Equations of motion
interacting and non-interacting scattering solutions

$$i\hbar \frac{d|\Psi^{\pm}(t)\rangle}{dt} = H|\Psi^{\pm}(t)\rangle \tag{113}$$

$$i\hbar \frac{d|\Psi_0^{\pm}(t)\rangle}{dt} = H_0|\Psi_0^{\pm}(t)\rangle \tag{114}$$

Møller wave operators
transform non-interacting to interacting scattering solutions

$$\Omega_{\pm} = \lim_{t\to\pm\infty} e^{iHt/\hbar} e^{-iH_0 t/\hbar} \tag{115}$$

$$|\Psi^{\pm}(t)\rangle = \Omega_{\pm}|\Psi_0^{\pm}(t)\rangle \tag{116}$$

Intertwining relation
leads to energy conservation in S

$$H\Omega_{\pm} = \Omega_{\pm} H_0 \tag{117}$$

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

$$P = |\langle \Psi_0^+(0)|\Omega_+^\dagger \Omega_- |\Psi_0^-(0)\rangle|^2 \tag{118}$$

$$P = |\langle \Psi_0^+(0)|S|\Psi_0^-(0)\rangle|^2 \tag{119}$$

$$S = \Omega_+^\dagger \Omega_- \tag{120}$$

$$[S, H_0] = 0 \tag{121}$$

Relation of S to dynamics

$$\langle \Psi_0^+(0)|S|\Psi_0^-(0)\rangle = \langle \Psi_0^+(0)|(I - 2\pi i \delta(E_+ - E_-)T(E_- + i\epsilon)|\Psi_0^-(0)\rangle \tag{122}$$

Transition operator

$$T(z) = V + V(z - H)^{-1}V \tag{123}$$

Lippmann Schwinger equation for the transition operator

$$T(z) = V + V(z - H_0)^{-1}T(z) \tag{124}$$

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

$$|\Psi^{\pm}(0)\rangle = |\mathbf{k}^{\pm}\rangle d\mathbf{k}\langle\mathbf{k}||\Psi_0^{\pm}(0)\rangle \tag{125}$$

$$|\mathbf{k}^{\pm}\rangle = |\mathbf{k}\rangle + (\mathbf{k}^2/2\mu - H \mp i\epsilon)^{-1}V|\mathbf{k}\rangle =$$
$$|\mathbf{k}\rangle + (\mathbf{k}^2/2\mu - H_0 \mp i\epsilon)^{-1}V|\mathbf{k}^{\pm}\rangle \tag{126}$$

Relation between scattering wave functions and transition operators

$$\langle\mathbf{k}'|T(\mathbf{k}^2/2\mu \pm i\epsilon)|\mathbf{k}\rangle = \langle\mathbf{k}'|V|\mathbf{k}^{\mp}\rangle \tag{127}$$

$$\langle\mathbf{k}'|T(\mathbf{k}^{2\prime}/2\mu \pm i\epsilon)|\mathbf{k}\rangle = \langle\mathbf{k}'^{\pm}|V|\mathbf{k}\rangle \tag{128}$$

Coordinate space representation of Lipppmann Schwinger equation

$$\langle\mathbf{r}|\mathbf{k}^{\pm}\rangle = \langle\mathbf{r}|\mathbf{k}^{\pm}\rangle - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{\mp ik|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')d\mathbf{r}'\langle\mathbf{r}'|\mathbf{k}\rangle \tag{129}$$

Large r limit of scattering wave functions
scattering amplitude

$$\lim_{r\to\infty}\langle\mathbf{r}|\mathbf{k}^{\pm}\rangle \to \frac{1}{(2\pi\hbar)^{3/2}}(e^{i\mathbf{k}\cdot\mathbf{r}/\hbar} + \frac{e^{ikr}}{r}F(k\hat{\mathbf{r}},\mathbf{k})) \tag{130}$$

Relation of transition operator to scattering amplitude

$$F(\mathbf{k}',\mathbf{k}) = -(2\pi)^2\hbar\mu\langle\mathbf{k}|T(E + i\epsilon)|\mathbf{k}\rangle \tag{131}$$

Differential cross section
removes dependence on free wave packets assuming that they are narrow

$$d\sigma = \frac{(2\pi)^4\hbar^2}{v} |\langle \mathbf{p}'_1, \mathbf{p}'_2 | T(E+i\epsilon) | \mathbf{p}_1, \mathbf{p}_2 \rangle|^2 \delta(E'-E)\delta(\mathbf{P}'-\mathbf{P}) d\mathbf{p}'_1 \mathbf{dp}'_2 \tag{132}$$

Exact form for transition rates
exact form of golden rule

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

$$\frac{2\pi}{\hbar} |\langle (\mathbf{p}'_1, \mathbf{p}'_2)^+ | V_d | \mathbf{p}_1, \mathbf{p}_2 \rangle|^2 \delta(E'-E)\delta(\mathbf{P}'-\mathbf{P}) d\mathbf{p}'_1 \mathbf{dp}'_2 \tag{133}$$

Scattering phase shifts

$$S = e^{2\imath\delta} \tag{134}$$

Partial wave representation of phase shifts

$$\langle \mathbf{k}' | S | \mathbf{k} \rangle = \langle \mathbf{k}' | e^{2i\delta} | \mathbf{k} \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y^l_m(\hat{\mathbf{k}}') e^{2i\delta_l(k)} Y^{l*}_m(\hat{\mathbf{k}}) \tag{135}$$

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

$$H = H_0 + V_1 + V_2 \qquad V_1 >> V_2 \tag{136}$$

$$T(z) \approx T_1(z) + \Omega^\dagger_{1+} V_2 \Omega_{1-} \tag{137}$$

Impossibility of constructing V from S.

$$\lim_{t\to\pm\infty} \| (A-I) e^{-iH_0 t/\hbar} |\Psi\rangle \| = 0 \qquad A^\dagger A = I \tag{138}$$

$$H' = A^\dagger H A = H_0 + V' \Leftrightarrow S' = S \tag{139}$$

Treatment of resonant decay

$$t_l \approx -\frac{1}{\pi\mu k}\frac{\Gamma/2}{E - E_b - \Delta E + i\Gamma/2} \tag{140}$$

$$\tau = \hbar/\Gamma \tag{141}$$

$$\Gamma = 2\pi\int\langle B|V_2|\mathbf{k}'\rangle d\mathbf{k}'\delta(\mathbf{k}'^2/2\mu - \mathbf{k}^2/2\mu)\langle\mathbf{k}'|V_1|B_1\rangle \tag{142}$$

Optical theorem
construct total cross section from forward scattering amplitude

$$S^\dagger S = I \tag{143}$$

$$Im(F(\mathbf{k},\mathbf{k})) = \frac{k}{4\pi\hbar}\sigma_t \tag{144}$$

$$\langle\mathbf{r}|\mathbf{k}^\pm\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_m^l(\hat{\mathbf{r}})\langle r|k^\pm, l\rangle Y_m^{l*}(\hat{\mathbf{k}}) \tag{145}$$

Partial wave Lippmann Schwinger equation

$$\langle r|k^-, l\rangle = \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}}(j_l(kr/\hbar) - i\frac{2\mu k}{\hbar^3}\int_0^\infty j_l(kr</\hbar)h_l^1(kr>/\hbar)r'^2dr'V(r')\langle r|k^-, l\rangle \tag{146}$$

Relation to partial wave transition operator

$$t_l(k,k,\mathbf{k}^2/2\mu + i\epsilon) = \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}}\int_0^\infty j_l(kr/\hbar)r'^2dr'V(r')\langle r|k^\pm, l\rangle \tag{147}$$

Relation to phase shifts

$$f_l(k) = -(2\pi)^2\mu\hbar t_l(k,k,\mathbf{k}^2/2\mu + i\epsilon) = \frac{4\pi\hbar}{k}e^{i\delta_l}\sin(\delta_l) \tag{148}$$

$$t_l(k,k,\mathbf{k}^2/2\mu + i\epsilon) = -\frac{1}{\pi\mu k}e^{i\delta_l}\sin(\delta_l) \tag{149}$$

$$\langle r|k^\pm, l\rangle \to \frac{4\pi(-i)^l}{(2\pi\hbar)^{3/2}}\frac{\hbar}{kr}e^{i\delta_l}\sin(\delta_l) \tag{150}$$

Identical particles

$$F(\mathbf{k}',\mathbf{k}) \to (F(\mathbf{k}',\mathbf{k}) \pm F(-\mathbf{k}',\mathbf{k})) \tag{151}$$

$$F(k,\theta) \to (F(k,\theta) \pm F(k,\pi-\theta)) \tag{152}$$