Scattering in the Interaction Representation

Scattering can be described either using the integral equation form of the Schrödinger equation, or as a time dependent process using the interaction picture. In this section, we discuss the interaction picture treatment in first order. The formulae are quite similar in $d = 1, 2$, or 3, so all three cases will be carried along. The Hamiltonian for the system is

$$H = \frac{\vec{P} \cdot \vec{P}}{2m} + V(\vec{X}),$$

where the potential is assumed to fall off rapidly at infinite distances. (The Coulomb potential in $d = 3$ is a borderline case.) The physical quantities describing scattering can be extracted from the matrix elements of U_I, calculated over an infinite time interval.

Basic Setup The matrix element takes the general form

$$< f|U_I(\infty, -\infty)|i >= (\mathcal{M}_{f,i})\, 2\pi\delta(\omega_f - \omega_i),$$

where the final energy is $E_f = \hbar\omega_f$, and the initial energy is $E_i = \hbar\omega_i$. The delta function for conservation of energy will be present in any order of perturbation theory, and is present in the exact matrix element of U_I. It is at first sight disconcerting to see a delta function in a matrix element of U_I. However, the matrix element being considered is between plane wave states of definite wave-vector, so this matrix element is not (yet) a probability amplitude. To obtain a probability amplitude, we must have physical, normalized states, both initial and final. Writing this in more detail, a true probability amplitude would be

$$< \Phi_f|U_I(\infty, -\infty)|\Phi_i >= \int d\vec{k}_f d\vec{k}_i < \Phi_f|\vec{k}_f >< \vec{k}_f|U_I(\infty, -\infty)|\vec{k}_i >< \vec{k}_i|\Phi_i >$$

This formula gives the probability amplitude for a transition from $|\Phi_i >$ at very early time to a state $|\Phi_f >$ at very late time. The delta function in the definite wave vector matrix element of U_I will be integrated over and the result is a finite probability amplitude. This approach is fundamental, but rather tedious to work with in practice. In its place a simple method which gives the same results for physical quantities is used. There are two main features to this approach. First, plane waves are still used instead of the physically correct wave packets, but the plane waves are made into normalizable states by imbedding the system in a large rectangular box with periodic boundary conditions. While this does make initial and final states normalizable, they are still spread throughout the system, unlike a true initial and final states which are free well before the collision and well after. This is mimicked by turning off the interaction before a large negative time $-T/2$, and after a large positive time $T/2$. We then have for the matrix element of U_I,

$$< \vec{k}_f|U_I(\infty, -\infty)|\vec{k}_i >= (\mathcal{M}_{f,i})\, \frac{2\sin(\omega_{f,i}T/2)}{\omega_{f,i}},$$

where $\omega_{f,i} = \omega_f - \omega_i = (E_f - E_i)/\hbar$. Defining

$$I(\omega, T) = \frac{2\sin(\omega T/2)}{\omega},$$

as a function of ω, $I(\omega, T)$ has a peak value of T at $\omega = 0$, and has its first zero at $\omega = 2\pi/T$. For any T, the integral of $I(\omega, T)$ from $\omega = -\infty$ to $+\infty$ is 2π, and

$$I(\omega, T) \to 2\pi\delta(\omega),\ as\ T \to \infty$$

Thus for large but finite T,$I(\omega, T)$ is a function with a sharp spike at $\omega = 0$, which is the condition of energy conservation. What constitutes "large T" depends on the frequencies in the problem. As a typical example, light in the optical range of wavelengths has $\omega \sim 10^{10} Hz$. Thus a time as short as $T \sim 1ns$ is in fact a very large value of T.

By putting the system in a box with periodic boundary conditions and restricting the interaction time to T, the matrix elements of U_I, which are probability amplitudes, are finite and well-behaved. Turning to probabilities themselves, we take the absolute square of the matrix elements of U_I, and sum over whatever final states are "of interest", this meaning what range of final momenta will be detected in the experiment. At this point we have

$$\mathcal{P} = \sum_f |\mathcal{M}_{f,i}|^2 (I(\omega, T))^2,\ \ \omega = \omega_f - \omega_i$$

where $\mathcal{P}$ is the probability, and the sum on final states f is restricted in a way appropriate to the experiment being performed. Now the function $(I(\omega, T))^2$ like $I(\omega, T)$ itself, has a very sharp spike at $\omega = 0$, but the height of the peak is T^2 instead of T. Mathematically, it is true that

$$I(\omega, T)^2 \to 2\pi T\delta(\omega)\ \ T \to \infty$$

For T large in the sense described above, the peak in $I(\omega, T)^2$ is so sharp that negligible error is cause by replacing $I(\omega, T)^2$ by $2\pi T\delta(\omega)$. But this implies that $\mathcal{P}$ grows linearly with T, so a quantity independent of T is obtained by dividing $\mathcal{P}$ by T. This is called the **transition rate** and has dimensions of frequency, i.e. it is a measure of the number of transitions/second. The formula for the rate is then

$$\mathcal{R} = \sum_f |\mathcal{M}_{f,i}|^2 2\pi\delta(\omega_f - \omega_i).$$

In an actual scattering situation, the rate is not yet the quantity of interest, since it is proportional to the number of particles which are incident. This is taken care of by dividing the rate by the incident current,

$$\sigma = \frac{\mathcal{R}}{J_{inc}}$$

It is worthwhile to note the dimensions of σ for $d = 1, 2, 3$. This is determined by the dimension of the current, since the rate always has dimensions of frequency. In the most familiar case of $d = 3$, the current has dimensions $1/area \cdot time$, while in $d = 2$ it has dimensions $1/length \cdot time$ and in $d = 1$ it has dimensions $1/time$. Thus in $d = 3$, the dimension of σ is area (crossection), in $d = 2$ it is length and in $d = 1$, σ is dimensionless.

The quantity σ depends on what final states are involved in the $\sum_f$. For example in $d = 3$, all energies may be accepted but the direction of the scattered particle may not be summed over. This would mean that outgoing particles are detected in individual small elements of solid angle. In this case one would have $d\sigma/d\Omega$, where $d\Omega$ refers to the element of solid angle. Summing over all directions of the scattered particle is done by integrating $d\sigma/d\Omega$ over solid angle, and gives the quantity known as the total cross section. Likewise in $d = 2$, if the angle of scattering is not summed, we would have $d\sigma/d\phi$ where ϕ is the angle of scattering. Finally in $d = 1$, one may differentiate between particles which are transmitted in the same direction of the incident particle, or reflected by $\sigma_{forward}$, or $\sigma_{backward}$.

First Order Calculation Let us now turn to the first order calculation in detail. The box normalized wave functions are

$$< \vec{x}|\vec{k} >= \frac{1}{\sqrt{\mathcal{V}}} \exp(i\vec{k} \cdot \vec{x}),$$

where the meaning of the "volume" $\mathcal{V}$ in the various dimensions is

$$\begin{array}{lll} \mathcal{V} = L & L_x L_y & L_x L_y L_z \\ d = 1 & d = 2 & d = 3 \end{array} .$$

The periodic boundary conditions mean that every component of wave vector is discrete,

$$k_x = \frac{2\pi n_x}{L_x}, etc.$$

Our first order calculation involves

$$U_I^{(1)} = \frac{-i}{\hbar} \int_1^2 V_I(t) dt,$$

where

$$V_I = \exp(\frac{iH_0 t}{\hbar}) V_S \exp(\frac{-iH_0 t}{\hbar}).$$

The matrix element of V_I is then

$$< \vec{k}_f|V_I|\vec{k}_i >=< \vec{k}_f| \exp(\frac{iH_0 t}{\hbar}) V_S \exp(\frac{-iH_0 t}{\hbar})|\vec{k}_i >$$

$$= \exp(i(\omega_f - \omega_i)t) < \vec{k}_f|V_S|\vec{k}_i > .$$

where

$$\hbar\omega_f = \frac{\hbar k_f^2}{2m}, \quad \hbar\omega_i = \frac{\hbar k_i^2}{2m} .$$

Going over to an infinite time interval we have for the matrix element of U_I,

$$< \vec{k}_f|U_I^{(1)}(\infty,-\infty)|\vec{k}_i >= \frac{-i}{\hbar} < \vec{k}_f|V_S|\vec{k}_i > 2\pi\delta(\omega_f-\omega_i),$$

so the rate becomes

$$\mathcal{R} = \sum_{k_f} |\frac{-i}{\hbar} < \vec{k}_f|V_S|\vec{k}_i > |^2 2\pi\delta(\omega_f-\omega_i).$$

In detail, the matrix element of V_S is

$$< \vec{k}_f|V_S|\vec{k}_i >= \frac{1}{\sqrt{\mathcal{V}}}\left(\int \exp(-i\vec{k}_f\cdot\ \vec{x})V_S(\vec{x})\exp(i\vec{k}_i\cdot\vec{x})\right)\frac{1}{\sqrt{\mathcal{V}}}$$

To express this result in terms of Fourier transforms, recall the definitions

$$f(\vec{x}) = \int \frac{d\vec{k}}{(2\pi)^d}\exp(i\vec{k}\cdot\vec{x})\tilde{f}(\vec{k}),$$

and

$$\tilde{f}(\vec{k}) = \int d\vec{x}\exp(-i\vec{k}\cdot\vec{x})f(\vec{x})$$

We see that the matrix element of V_S can be expressed in terms of the Fourier transform of V_S,

$$< \vec{k}_f|V_S|\vec{k}_i >= \tilde{V}_S(\vec{k}_f-\vec{k}_i)$$

Sum on Final States Now we turn to the sum on final states. At present, we have a sum over the discrete wave vectors in our periodic box. However, when the size of the box goes to infinity, the sum will go over to an integral times a characteristic factor. To see what the factor is, we first write out the forms for the wave vectors for the case of $d = 3$. We have

$$k_x = \frac{2\pi n_x}{L_x},\quad k_y = \frac{2\pi n_y}{L_y},\quad k_z = \frac{2\pi n_z}{L_z}$$

so the spacing between success values of the wave vector components is

$$\Delta k_x = \frac{2\pi}{L_x},\quad \Delta k_y = \frac{2\pi}{L_y},\quad \Delta k_z = \frac{2\pi}{L_z}'$$

so $(L_x/2\pi)\Delta k_x = 1$, etc for k_y, and k_z. Rewriting the sum on discrete wave vectors and using the (Riemann) definition of integral, we have that a sum over wave vectors becomes for $d = 3$,

$$\frac{L_x}{2\pi}\frac{L_y}{2\pi}\frac{L_z}{2\pi}\sum_{k_x,k_y,k_z} f(\vec{k})\Delta k_x\Delta k_y\Delta k_z \to \frac{\mathcal{V}}{(2\pi)^3}\int d\vec{k}f(\vec{k}),$$

where we have basically inserted “1” in the sum on final wave vectors. Applying this to our rate, we have

$$\mathcal{R} \to \frac{\mathcal{V}}{(2\pi)^3} \int d\vec{k}\, |\frac{1}{\sqrt{\mathcal{V}}} \tilde{V}_S(\vec{k}_f - \vec{k}_i) \frac{1}{\sqrt{\mathcal{V}}}|^2 2\pi\delta(\omega_f - \omega_i)$$

We see that the factors of $\mathcal{V}$ associated with the final particle cancel. Those associated with the initial particle will also cancel when we divide by the current. We will perform that step after treating the energy conservation delta function.

Energy Conservation Delta Function Let us first define the ω's. We have

$$\omega_f = \frac{1}{\hbar}\frac{(\hbar k_f)^2}{2m} = \frac{\hbar}{2m}k_f^2, \quad \omega_i = \frac{\hbar}{2m}k_i^2$$

Using these definitions, we can rewrite the delta function as

$$\delta(\omega_f - \omega_i) = \frac{2m}{\hbar}\delta(k_f^2 - k_i^2)$$

Now in all cases, we will integrate over the magnitude of the final wave vector. The factors from the integration weight vary as the dimension of our problem changes. For one dimensional scattering, we have

$$dk_f \delta(\omega_f - \omega_i) = (\frac{2m}{\hbar})\frac{dk_f}{2k_i}(\delta(k_f - k_i) + \delta(k_f + k_i)).$$

In this one dimensional case, if final states are accepted from $k_f = -\infty$ to 0, only the reflected scattering is included, while if final states are accepted from $k_f = 0$ to $+\infty$, only transmitted scattering is included, and of course both can be included by integrating $-\infty$ to $+\infty$. For two dimensional scattering, we have

$$k_f dk_f \delta(\omega_f - \omega_i) = (\frac{2m}{\hbar})\frac{dk_f^2}{2}\delta(k_f^2 - k_i^2)$$

and finally for three dimensions, we obtain

$$k_f^2 dk_f \delta(\omega_f - \omega_i) = (\frac{2m}{\hbar})k_f\frac{dk_f^2}{2}\delta(k_f^2 - k_i^2)$$

In all cases, after the integration over the magnitude of k_f is completed, we have $k_f = k_i$, and there is a net factor involving k_i which can be written as

$$\frac{m}{\hbar k_i}(k_i)^{d-1}.$$

Note that the ratio $m/\hbar k_i$ is just the velocity of the incident particle.

Incident Current and Final Results Finally, we note that the incident current is

$$J_{inc} = \frac{\hbar}{2mi}[\Psi^* \partial_z \Psi - (\partial_z \Psi^*)\Psi]$$
$$= \frac{\hbar |k_i|}{m} \frac{1}{\mathcal{V}}.$$

(The incident direction is usually taken to be the z-direction.) Dividing by the current will remove the volume factors associated with the incident particle.

We can now summarize the results in $d = 1, 2, 3$. For $d = 1$ we have

$$\sigma_{forward} = |\frac{1}{\hbar}\tilde{V}_S(0)|^2 (\frac{m}{\hbar k_i})^2$$

$$\sigma_{backward} = |\frac{1}{\hbar}\tilde{V}_S(-2k_i)|^2 (\frac{m}{\hbar k_i})^2.$$

For $d = 2$ we have

$$\frac{d\sigma}{d\phi} = \frac{1}{2\pi}|\frac{1}{\hbar}\tilde{V}_S(\vec{k}_f - \vec{k}_f)|^2 k_i (\frac{m}{\hbar k_i})^2$$

Finally in $d = 3$ we have

$$\frac{d\sigma}{d\Omega} = \frac{1}{(2\pi)^2}|\frac{1}{\hbar}\tilde{V}_S(\vec{k}_f - \vec{k}_f)|^2 k_i^2 (\frac{m}{\hbar k_i})^2 = (\frac{m}{2\pi\hbar^2})^2 |\tilde{V}_S(\vec{k}_f - \vec{k}_f)|^2 \quad (1)$$

The 2π factors in these formulas comes from the 2π which accompanies the energy conservation delta function, and the $1/(2\pi)^d$ that comes into the sum on final states. It is easily checked that the various scattering quantities have dimensions $(length)^{d-1}$. These results are of course for first order scattering, known as the Born Approximation. This is a good approximation for high energy scattering, where the kinetic energies are large compared to the potential. Calculations in the Born Approximation are very easy-all that is needed is the Fourier transform of V_S.

0.1 Yukawa Potential in Three Dimensions

A potential of the form

$$V_S = \frac{\lambda}{r}\exp(-\alpha r)$$

a so-called Yukawa potential, is an important case. Note that for $\alpha = 0$, we obtain a Coulombic potential. Let us calculate $\tilde{V}_S(\vec{q})$, which is given by

$$\tilde{V}_S(\vec{q}) = \int d^3r \exp(i\vec{q}\cdot\vec{r}) V_S(r)$$

Let us choose our coordinate system so that $\vec{q}$ is aligned along the z axis. This makes it easy to do the angle integrations. We have

$$\exp(i\vec{q}\cdot\vec{r}) = \exp(iqz) = \exp(iqr\cos\theta).$$

The angular part of our integral is then

$$\int \sin\theta d\theta d\phi \exp(iqr\cos\theta)$$

The ϕ integration gives a factor of 2π, and we have

$$2\pi \int_{-1}^{1} d(\cos\theta) \exp(iqr\cos\theta) = 4\pi \frac{\sin(qr)}{qr}$$

Returning to $\tilde{V}_S(\vec{q})$, we now have

$$\tilde{V}_S(\vec{q}) = \int_0^\infty r^2 dr (\frac{4\pi \sin(qr)}{qr}) \frac{\lambda}{r} \exp(-\alpha r) = \frac{4\pi\lambda}{q} \int_0^\infty dr \sin(qr) \exp(-\alpha r)$$

The radial integral is easy to do. We have

$$\int_0^\infty dr \frac{1}{2i} (\exp(iqr) - \exp(-iqr)) \exp(-\alpha r) = \frac{1}{2i} [\frac{1}{\alpha - iq} - \frac{1}{\alpha + iq}] = \frac{q}{\alpha^2 + q^2}$$

We finally have

$$\tilde{V}_S(\vec{q}) = \frac{4\pi\lambda}{\alpha^2 + q^2}$$

Making use of Eq.(1) we have

$$\frac{d\sigma^{(1)}}{d\Omega_f} = (\frac{2m}{\hbar^2})^2 \frac{\lambda^2}{(\alpha^2 + q^2)^2}$$

To see what sort of angular distribution this implies, we recall that

$$q^2 = (\vec{k}_f - \vec{k}_i) \cdot (\vec{k}_f - \vec{k}_i)$$

Now by energy conservation, $|\vec{k}_f| = |\vec{k}_i| \equiv k$, so

$$q^2 = 2k^2(1 - \cos\theta)$$

where the angle θ is the *angle of scattering*, i.e. the angle between $\vec{k}_f$ and $\vec{k}_i$. Using the formula

$$2(1 - \cos\theta) = \sin^2(\theta/2),$$

we finally have

$$\frac{d\sigma^{(1)}}{d\Omega_f} = (\frac{2m}{\hbar^2})^2 \frac{\lambda^2}{(\alpha^2 + k^2 \sin^2(\theta/2))^2}$$

This formula is the Born approximation for a Yukawa potential. If $\alpha = 0$, it reduces to a Coulombic potential. The Coulombic case is of course equivalent to *Rutherford Scattering*. A huge amount of information on Rutherford scattering is available on the web-just Google "Rutherford Scattering".

The Born approximation is valid the potential is weak compared to the kinetic energy of the particle. The energy of the incident particle (and the scattered particle) is $(\hbar k)^2/2m$. To make a rough estimate, let is evaluate the potential at $r \sim \alpha$. Then our criterion is approximately

$$\lambda\alpha << \frac{(\hbar k)^2}{2m},$$

so the Born approximation is clearly a good one at high energy.