I offer here some background for Chapter 7 of J. J. Sakurai, *Modern Quantum Mechanics*.

## 1 The problem

We consider the evolution of a system under a hamiltonian

\[ H(t) = H_0 + V_S(t) . \] (1)

Here \( H_0 \) is simple enough that we can solve exactly for its eigenstates, while \( V_S(t) \) is a perturbing interaction with the form

\[ V_S(t) = V g(t) . \] (2)

We use the function \( g(t) \) as a device to turn the interaction off for large positive times and large negative times. For times in a long interval about \( t = 0 \) we take \( g(t) = 1 \). We define the effective time that the interaction is on by

\[ T = \int dt \ |g(t)|^2 . \] (3)

We are interested in what happens in the limit \( T \to \infty \).

We will use the interaction picture based on the unperturbed hamiltonian \( H_0 \). In this picture, the state of the system is time independent far in the past and far in the future, when \( g(t) = 0 \). We suppose that the system starts in a state \( |\psi_I\rangle \) far in the past and we seek the probability that it will be found to be in a state \( |\psi_F\rangle \) far in the future. We take these states to be eigenstates of \( H_0 \):

\[ H_0 |\psi_I\rangle = E_I |\psi_I\rangle , \]
\[ H_0 |\psi_F\rangle = E_F |\psi_F\rangle . \] (4)
We consider two examples of this, scattering of a single nonrelativistic particle from a potential and scattering involving absorption or emission of photons from atoms.

1.1 Scattering from a potential

In this class of examples, we will consider scattering of a single, spinless particle from a fixed potential $V(\vec{x})$. This is the simplest example of scattering theory.

For the fixed potential case, the hamiltonian is

$$H(t) = H_0 + V_S(t) .$$

where

$$H_0 = \frac{\vec{p}^2}{2m}$$

and

$$V_S(t) = V g(t) .$$

Here $V$ is an operator given by

$$V = V(\vec{x}) .$$

where $V(\vec{x})$ is a function of the position operator $\vec{x}$ of the particle.

We use the interaction picture based on the unperturbed hamiltonian $H_0$ and suppose that the system starts far in the past in a momentum eigenstate

$$|\psi_I\rangle = |\vec{k}_I\rangle ,$$

where $\vec{k}_I$ is along the $z$-axis. We ask for the amplitude for the system to wind up far in the future in a different momentum eigenstate

$$|\psi_F\rangle = |\vec{k}_F\rangle .$$

Thus

$$E_I = \frac{\vec{k}_I^2}{2m} ,$$

$$E_F = \frac{\vec{k}_F^2}{2m} .$$
1.2 Scattering with photons

In our second example, an electron interacts with a force center and also interacts with a photon. The electron together with the force center is then an “atom” if the electron is in a bound state or an ionized atom if it is in an unbound state. The hamiltonian is

\[ H(t) = H_0 + V_S(t) . \]  

(12)

where

\[ H_0 = \frac{\vec{p}^2}{2m} + V_0(r) + H_\gamma \]  

(13)

where \( V_0(r) \) is the binding potential. The simplest example is a hydrogen atom, for which \( V_0(r) = -e^2/r \). The last term is the hamiltonian for free photons, with

\[ H_\gamma |\vec{k},\lambda \rangle = \omega(k) |\vec{k},\lambda \rangle . \]  

(14)

Here \( \omega(k) = |\vec{k}| \) in our units with \( c = 1 \).

The perturbation is then

\[ V_S(t) = V g(t) . \]  

(15)

Here \( V \) is an operator given by

\[ V = \frac{e}{m} \vec{A}(\vec{x}, 0) \cdot \vec{p} . \]  

(16)

The argument \( \vec{x} \) of \( \vec{A}(\vec{x}, t) \) is the position of the electron. We set the time to 0 in order to write the quantum field in the Schrödinger picture. Recall that the matrix element of \( \vec{A}(\vec{x}, 0) \) between the vacuum and a photon state is

\[ \langle 0 | \vec{A}(\vec{x}, 0) |\vec{k},\lambda \rangle = \frac{1}{2\pi\sqrt{\omega(k)}} \bar{\epsilon}(\vec{k}, \lambda) e^{i\vec{k} \cdot \vec{x}} , \]  

\[ \langle \vec{k},\lambda | \vec{A}(\vec{x}, 0) |0 \rangle = \frac{1}{2\pi\sqrt{\omega(k)}} \epsilon(\vec{k}, \lambda)^* e^{-i\vec{k} \cdot \vec{x}} . \]  

(17)

2 First order perturbation theory

Now we are ready for perturbation theory. We will start with first order perturbation theory. In the following section, we will switch to all order perturbation theory, which is a bit more complicated but also more interesting.
The amplitude to find the system in state $|\psi_F\rangle$ at a time $t$ far in the future is

$$
\langle \psi_F | U_I^{(1)}(T; \infty, -\infty) | \psi_I \rangle = -i \int dt \langle \psi_F | V_I(t) | \psi_I \rangle = -i \langle \psi_F | V_I \rangle \int dt \ e^{i(E_F - E_I) t} g(t)
$$

(18)

The argument $T$ here reminds us that we are using the function $g(t)$, which will eventually become just 1 in the limit $T \rightarrow \infty$. The function $\tilde{g}(\omega')$ is the Fourier transform of $g(t)$,

$$
\tilde{g}(\omega) = \int dt \ e^{i\omega t} g(t) ,
\text{ and } g(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{g}(\omega).
$$

(19)

The probability to find the system in state $|\psi_F\rangle$ at a time $t$ far in the future is

$$
|\langle \psi_F | U_I^{(1)}(T; \infty, -\infty) | \psi_I \rangle|^2 = |\langle \psi_F | V_I | \psi_I \rangle|^2 |\tilde{g}(E_F - E_I)|^2 .
$$

(20)

Recall that $g(t)$ is very flat as a function of time. It is almost 1 for a long time. In particular, $g(0) = 1$. Since $g(t)$ is very flat, $\tilde{g}(\omega')$ as a function of frequency is very sharply peaked near $\omega' = 0$. That is, for any function $h(\omega)$ we will have

$$
\int d\omega \ \tilde{g}(\omega) h(\omega) \sim h(0) \int d\omega \ \tilde{g}(\omega) = 2\pi h(0)g(0) = 2\pi h(0).
$$

(21)

That is,

$$
\tilde{g}(\omega) \sim 2\pi \delta(\omega)
$$

(22)

for $T \rightarrow \infty$. Thus in Eq. (18) we have

$$
\lim_{T \rightarrow \infty} \langle \psi_F | U_I^{(1)}(T; \infty, -\infty) | \psi_I \rangle = 2\pi \delta(E_F - E_I) (-i) \langle \psi_F | V_I | \psi_I \rangle .
$$

(23)

If we simply square the amplitude to get a probability, we get the square of a delta function, which doesn’t make much sense. However, in Eq. (20) we
have
\[
\int d\omega \ |\tilde{g}(\omega)|^2 h(\omega) \sim h(0) \int d\omega \ |\tilde{g}(\omega)|^2 = 2\pi h(0) \int dt \ |\tilde{g}(t)|^2 = 2\pi h(0)T .
\] (24)

That is
\[
|\tilde{g}(\omega)|^2 \sim 2\pi \delta(\omega) T ,
\] (25)

Thus
\[
\lim_{T \to \infty} \frac{1}{T} |\langle \psi_F | U_I^{(1)}(T; \infty, -\infty) | \psi_I \rangle|^2 = 2\pi \delta(E_F - E_I) |\langle \psi_F | V | \psi_I \rangle|^2 .
\] (26)

3 Scattering in perturbation theory

In this section, we use time dependent perturbation theory to set up scattering theory and, at the same time, to generate the perturbative expansion of the scattering amplitude. Starting from state $|\psi_I\rangle$ in the distant past, the amplitude to find the system in state $|\psi_F\rangle$ at a time far in the future is
\[
\langle \psi_F | U_I(T; \infty, -\infty) | \psi_I \rangle .
\] (27)

Recall that $U_I$ has a perturbative expansion in powers of $V$,
\[
\langle \psi_F | U_I(T; \infty, -\infty) | \psi_I \rangle = \langle \psi_F | \psi_I \rangle + \sum_{n=1}^{\infty} \langle \psi_F | U_I^{(n)}(T; \infty, -\infty) | \psi_I \rangle .
\] (28)

Recall also that
\[
U_I^{(n)}(T; \infty, -\infty) = (-i)^n \int_{-\infty}^{\infty} d\tau_n \cdots \int_{-\infty}^{\tau_3} d\tau_2 \int_{-\infty}^{\tau_2} d\tau_1 \times V_I(\tau_n) \cdots V_I(\tau_2) V_I(\tau_1) .
\] (29)

Let us change integration variables to $t_j$ defined by
\[
\tau_1 = t_1 , \\
\tau_2 = t_1 + t_2 , \\
\vdots \\
\tau_n = t_1 + \cdots + t_n .
\] (30)
Then

\[ U_1^{(n)}(T; \infty, -\infty) = (-i)^n \int_{-\infty}^{\infty} dt_1 \int_{0}^{\infty} dt_2 \cdots \int_{0}^{\infty} dt_n \times V_1(t_1 + \cdots + t_n) \cdots V_1(t_1 + t_2) V_1(t_1) . \]  

(31)

Now we take the \( \langle \psi_F | \cdots | \psi_1 \rangle \) matrix element of this and insert intermediate states that are eigenstates of \( H_0 \). That is, we use

\[ 1 = \sum_{\psi} \langle \psi | \psi \rangle . \]  

(32)

We use

\[ \langle \psi_J | V_1(t_1 + \cdots + t_J) | \psi_{J-1} \rangle = \langle \psi_J | V | \psi_{J-1} \rangle e^{i(E_J - E_{J-1})(t_1 + \cdots + t_J)} g(t_1 + \cdots + t_J) . \]  

(33)

After accounting for cancellations in the exponent, we get

\[ \langle \psi_F | U_1^{(n)}(T; \infty, -\infty) | \vec{k}_1 \rangle = (-i)^n \int_{-\infty}^{\infty} dt_1 \int_{0}^{\infty} dt_2 \cdots \int_{0}^{\infty} dt_n \times \sum_{\psi_1} \sum_{\psi_2} \cdots \sum_{\psi_n-1} \times \langle \psi_F | V | \psi_{n-1} \rangle \cdots \langle \psi_2 | V | \psi_1 \rangle \langle \psi_1 | V | \psi_1 \rangle \times e^{i(E_F - E_{n-1})t_n} \cdots e^{i(E_F - E_1)t_2} e^{i(E_F - E_1)t_1} \times g(t_1 + \cdots + t_n) \cdots g(t_1 + t_2) g(t_1) . \]  

(34)

We can now perform the time integrals. For all of the times \( t_J \) except \( t_1 \), we have an integral from 0 to \( \infty \):

\[ \int_{0}^{\infty} dt_J \ e^{i(E_F - E_{J-1})t_J} . \]  

(35)

The integrand comes with some factors of \( g \), which tell us that the integral is to be cut off at very large positive \( t_J \). For instance, we can start with the integration over \( t_n \) at a fixed value of \( t_1, \ldots, t_{n-1} \). The factor \( g(t_1 + \cdots + t_n) \) provides a cutoff at large \( t_n \). We just replace this \( g \) by

\[ g(t_1 + \cdots + t_n) \to e^{-\epsilon t_n} . \]  

(36)
Next, we perform the integration over $t_{n-1}$ in the same fashion. In each case, we replace the cutoff provided by the factors $g$ by an exponential cutoff, giving

$$
\int_0^\infty dt_j \ e^{i(E_F - E_{J-1} + i\epsilon) t_j} = \frac{i}{E_F - E_{J-1} + i\epsilon} .
$$

(37)

Here we understand that we are supposed to take the limit $\epsilon \to 0$. For the integration over $t_1$, we integrate from $-\infty$ to $+\infty$. This gives the Fourier transform $\tilde{g}(E_F - E_I)$ of $g(t)$:

$$
\int_{-\infty}^{\infty} dt_1 \ e^{i(E_F - E_I) t_1} g(t_1) = \tilde{g}(E_F - E_I) .
$$

(38)

In the limit $T \to \infty$, we use Eq. (22) and get

$$
\int_{-\infty}^{\infty} dt_1 \ e^{i(E_F - E_I) t_1} = 2\pi \delta(E_F - E_I) .
$$

(39)

We will take the limit in this form, but we will need to remember at some point that $2\pi \delta(E_F - E_I)$ should really have been $\tilde{g}(E_F - E_I)$.

Thus we obtain, in the $T \to \infty$ limit,

$$
\langle \psi_F | U_1^{(n)}(\infty, -\infty) | \psi_I \rangle = 2\pi \delta(E_F - E_I) \ (-i)^n \sum_{\psi_1} \sum_{\psi_2} \cdots \sum_{\psi_{n-1}}
$$

$$
\times \left\langle \psi_F | V | \psi_{n-1} \right\rangle \frac{i}{E_F - E_{n-1} + i\epsilon} \cdots
$$

$$
\times \left\langle \psi_2 | V | \psi_1 \right\rangle \frac{i}{E_F - E_1 + i\epsilon} \left\langle \psi_1 | V | \psi_I \right\rangle .
$$

(40)

This applies for $n \geq 1$.

4 Factoring out energy conservation

We can write this in a useful form,

$$
\langle \psi_F | U_1^{(n)}(\infty, -\infty) | \psi_I \rangle = 2\pi \delta(E_F - E_I) \ (-i) \langle \psi_F | T^{(n)} | \psi_I \rangle
$$

(41)
for $n \geq 1$, where

$$
\langle \psi_F | T^{(n)} | \psi_I \rangle = \frac{i (-i)^n}{2} \sum_{\psi_1} \sum_{\psi_2} \cdots \sum_{\psi_{n-1}} \\
\times \langle \psi_F | V | \psi_{n-1} \rangle \frac{i}{E_F - E_{n-1} + i\epsilon} \\
\times \langle \psi_{n-1} | V | \psi_1 \rangle \frac{i}{E_F - E_1 + i\epsilon} \langle \psi_1 | V | \psi_I \rangle .
$$

We can write this in a more compact fashion by eliminating the sums over intermediate states,

$$
\langle \psi_F | T^{(n)} | \psi_I \rangle = \langle \psi_F | V \frac{1}{E_F - H_0 + i\epsilon} \cdots V \frac{1}{E_F - H_0 + i\epsilon} \psi_I \rangle .
$$

Here there are $n$ factors of $V$.

Let us define

$$
T = \sum_{n=1}^{\infty} T^{(n)} .
$$

That is

$$
T(E) = V + V \frac{1}{E - H_0 + i\epsilon} V + \cdots .
$$

We also define

$$
\langle \psi_F | S | \psi_I \rangle = \langle \psi_F | U_1(\infty, -\infty) | \psi_I \rangle \\
= \langle \psi_F | \psi_I \rangle + \sum_{n=1}^{\infty} \langle \psi_F | U_1^{(n)}(\infty, -\infty) | \psi_I \rangle .
$$

Then

$$
\langle \psi_F | S | \psi_I \rangle = \langle \psi_F | \psi_I \rangle + 2\pi \delta(E_F - E_i)(-i)\langle \psi_F | T(E_F) | \psi_I \rangle .
$$

One calls $S$ the scattering operator and $\langle \psi_F | S | \psi_I \rangle$ the S-matrix. Then $\langle \psi_F | T(E_F) | \psi_I \rangle$ is the T-matrix. They differ in three ways: the S-matrix has a no-scattering term; there is an energy conserving delta function in the S-matrix that is not included in the T-matrix; and we factor a $(-i)$ out of the T-matrix, so that its perturbative expansion starts at $V$.

Notice that $T(E)$ as defined by its perturbative expansion (45) is an operator that depends on an energy variable $E$. In the definition (47), we take $E$ to be the energy of the final state, $E_F$, which equals also the energy of the initial state $E_i$. However, the definition (45) does not involve any particular states, so $T(E)$ is defined for any $E$. 
5 The cross section

In this section we relate the scattering amplitude to the cross section for each of our two cases, scattering of a nonrelativistic particle from a potential and scattering involving atoms and photons.

5.1 Scattering from a potential

The differential probability to get a given final state characterized by $\vec{k}_F$ (with $\vec{k}_F \neq \vec{k}_I$) is

$$dP(\vec{k}_I \to \vec{k}_F) = d\vec{k}_F \left| \langle \vec{k}_F | U(0, T; \infty, -\infty) | \vec{k}_I \rangle \right|^2 . \quad (48)$$

Here we need to be careful about the $T \to \infty$ limit. We write this as

$$dP(\vec{k}_I \to \vec{k}_F) = |\tilde{g}(E_F - E_I)|^2 d\vec{k}_F \left| \langle \vec{k}_F | T | \vec{k}_I \rangle \right|^2 . \quad (49)$$

We use Eq. (25) to replace

$$|\tilde{g}(E_F - E_I)|^2 \sim 2\pi \delta(E_F - E_I) T . \quad (50)$$

Thus

$$dP(\vec{k}_I \to \vec{k}_F) = 2\pi \delta(E_F - E_I) T d\vec{k}_F \left| \langle \vec{k}_F | T | \vec{k}_I \rangle \right|^2 . \quad (51)$$

That is, our probability is proportional to $T$, which is why we needed to beware of taking the limit $T \to \infty$. However, if we divide by $T$, we can take a limit,

$$\frac{1}{T} dP(\vec{k}_I \to \vec{k}_F) = 2\pi \delta(E_F - E_I) d\vec{k}_F \left| \langle \vec{k}_F | T | \vec{k}_I \rangle \right|^2 . \quad (52)$$

We also divide by the flux $F$ of incoming particles, that is, the number of incoming particles that cross a unit area per unit time. For an incoming plane wave, the number of particles per unit volume is

$$\rho = \left| \langle \vec{x} | \vec{k}_I \rangle \right|^2 = \frac{1}{(2\pi)^3} . \quad (53)$$

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$^3$Note that we could normalize our plane wave states with $|\vec{k}\rangle_V = V^{-1/2} |\vec{k}\rangle$ where $V$ is any number we like with dimensions of volume, for example $1\text{ m}^3$. Then $1 = V \int d\vec{k} \langle \vec{k} | V | \vec{k} \rangle_V$, so $|\vec{k}\rangle_V$ is dimensionless. In that case, we the number of particles per unit volume is $\rho = 1/(2\pi)^3 V$, which has the proper dimension $1/V$. If we do this, the factors of $V$ will cancel in a cross section. Normally, we just leave out the factors of $V$. 
The velocity of the particle is
\[ v = \frac{|\vec{k}_1|}{m}. \tag{54} \]

Thus the flux of incoming particles is
\[ F = \rho v = \frac{|\vec{k}_1|}{(2\pi)^3 m}. \tag{55} \]

One defines the differential cross section as
\[ d\sigma(\vec{k}_1 \rightarrow \vec{k}_F) = \frac{1}{FT} dP(\vec{k}_1 \rightarrow \vec{k}_F). \tag{56} \]

Thus
\[ d\sigma(\vec{k}_1 \rightarrow \vec{k}_F) = 2\pi \delta(E_F - E_I) \frac{(2\pi)^3 m}{|\vec{k}_1|} |\langle \vec{k}_F | T | \vec{k}_1 \rangle|^2. \tag{57} \]

We can simplify the result a bit by writing
\[ d\vec{k}_F \delta(E_F - E_I) = k_F^2 dk_F \delta \left( \frac{k_F^2}{2m} - E_I \right) d\Omega_F = mk_F d\Omega_F. \tag{58} \]

Since \( E_I = \frac{k_I^2}{2m} \), we have \( k_F \equiv |\vec{k}_F| = |\vec{k}_1| \equiv k_1 \). Then
\[ \frac{d\sigma(\vec{k}_1 \rightarrow \vec{k}_F)}{d\Omega_F} = (2\pi)^4 m^2 |\langle \vec{k}_F | T | \vec{k}_1 \rangle|^2. \tag{59} \]

Thus we need to calculate \( \langle \vec{k}_F | T | \vec{k}_1 \rangle \) and we immediately get the cross section.

Note the normalization of states that we have been using, following Sakurai:
\[ \langle \vec{x} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{x}}. \tag{60} \]

Thus there is a factor \((2\pi)^{-6}\) coming from the normalization of our plane wave states.
5.2 Photons

Either of the incoming or the outgoing particle could also be a photon. If the incoming particles are photons, the velocity of the photons is \( c = 1 \) and the flux of incoming particles is

\[
F = \rho c = \frac{1}{(2\pi)^3} \text{ (photons)}.
\]  

(61)

If the outgoing particle is a photon, then

\[
d\vec{k}_F \delta(E_F - E_I) = k_F^2 dk_F \delta(k_F - E_I) d\Omega_F = k_F^2 d\Omega_F \text{ (photons)}.
\]  

(62)

Thus a more general form of the cross section formula is

\[
\frac{d\sigma((\vec{k}_I, s_I) \rightarrow (\vec{k}_F, s_F))}{d\Omega_F} = (2\pi)^4 \frac{k_F^2}{v_I v_F} |\langle \vec{k}_F, s_F | \mathcal{T} | \vec{k}_I, s_I \rangle|^2
\]  

(63)

where

\[
v_I = \begin{cases} 
  k_I/m & \text{nonrel.} \\
  1 & \text{photon}
\end{cases}
\]

(64)

and

\[
v_F = \begin{cases} 
  k_F/m & \text{nonrel.} \\
  1 & \text{photon}
\end{cases}
\]

(65)

Here I have included a spin (or polarization) index \( s_I \) for the initial particle and another index \( s_F \) for the final particle. For a spin zero particle, there is no spin index. For an electron, there is an index with values \( \pm 1/2 \). For a photon there is a polarization index, usually called \( \lambda \), that takes two values.

6 Lowest order perturbation theory

At first order, \( \mathcal{T} = V \), so (for scattering from a potential)

\[
\langle \vec{k}_F | \mathcal{T}^{(1)} | \vec{k}_I \rangle = \langle \vec{k}_F | V | \vec{k}_I \rangle = (2\pi)^{-3} \int d\vec{x} \ e^{-i(k_F - k_I) \cdot \vec{x}} \ V(\vec{x}) .
\]  

(66)

We can also apply lowest order perturbation theory to the case in which a photon with momentum \( \vec{k} \) and polarization \( \lambda \) is absorbed by the electron in a bound state of a hydrogen atom, ionizing the atom. Let us call the
initial atom state $|1\rangle$ and the final ionized state $|\vec{k}_F\rangle$, as in the notes on time dependent perturbation theory. Thus we seek $\langle \vec{k}_F | T^{(1)} | 1; \vec{k}, \lambda \rangle$.

$$
\langle \vec{k}_F | T^{(1)} | 1; \vec{k}, \lambda \rangle = \langle \vec{k}_F | V | 1; \vec{k}, \lambda \rangle \\
= \langle \vec{k}_F | \frac{e}{m} \vec{A}(\vec{x}, 0) \cdot \vec{p} | 1; \vec{k}, \lambda \rangle \\
= \frac{e}{m} \frac{1}{2\pi \sqrt{\omega(k)}} \vec{e}(\vec{k}, \lambda) \cdot \langle \vec{k}_F | e^{i\vec{k}\cdot\vec{x}} \vec{p} | 1 \rangle
$$

(67)

From here, we can proceed as in our notes on time ordered perturbation theory.

**Exercise 6.1** Using first order perturbation theory, find the differential cross section $d\sigma/d\Omega_F$ for scattering a nonrelativistic particle of mass $m$, charge $e$, and momentum $k\hat{z}$ from a repulsive potential

$$
V(r) = \frac{e^2}{r}.
$$

(68)

State your result as a function of $k$ and the scattering angle $\theta$.

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### 7 Higher order perturbation theory

At second order,

$$
T^{(2)}(E_F) = V \left( \frac{1}{E_F - H_0 + i\epsilon} \right) V ,
$$

(69)

so

$$
\langle \psi_F | T^{(2)}(E_F) | \psi_1 \rangle = \sum_{\psi_1} \langle \psi_F | V | \psi_1 \rangle \frac{1}{E_F - E_1 + i\epsilon} \langle \psi_1 | V | \psi_1 \rangle .
$$

(70)

Notice that the perturbative expansion for $T$ is much simpler than the expansion for energy levels using time independent perturbation theory. With
more terms, we have

\[
\mathcal{T}(E_F) = V \\
+ V \frac{1}{E_F - H_0 + i\epsilon} V \\
+ V \frac{1}{E_F - H_0 + i\epsilon} V \frac{1}{E_F - H_0 + i\epsilon} V \\
+ \cdots.
\]

(71)

8 Decaying states

Recall from the notes on time dependent perturbation theory that an excited state of an atom can decay to a lower energy state by emitting a photon. We saw there how to calculate the decay rate \(\Gamma\) in first order perturbation theory. But, if the state decays, how can it be an energy eigenstate? Clearly, it isn’t. But then, what is it?

We can get some insight into these questions by using higher order perturbation theory. Let’s start with an atom in state \(|1\rangle\), which we take here to be the atom ground state, with energy \(E_1\). Suppose that the atom has an excited state \(|2\rangle\) with energy \(E_2\). This is a genuine eigenstate of \(H_0\), the atom hamiltonian not including interactions with photons. Now suppose that we start with the ground state plus a photon, \(|1; \mathbf{k}, \lambda\rangle\). Suppose that \(\omega(\mathbf{k}) \approx E_2 - E_1\). Then we get to state \(|2, 0\rangle\), with the atom in state 2 and no photon. Or, in any case, we almost get to this state. But the state can decay to \(|1; k', \lambda'\rangle\) consisting of the atom in its ground state plus a final state photon with momentum \(k'\) and polarization \(\lambda'\). We need \(\omega(k') = \omega(k)\) in order to conserve energy. What is the scattering amplitude for this reaction?

This can’t happen at first order in \(V\) but it can at second order.\(^4\) The

\(^{4}\)Actually, the atom can absorb one photon and emit another photon at first order in \(V\) using the \(\hat{A}^2\) term in \(V\). This is a small effect in the present context so we ignore it.
second order contribution is

$$\langle 1; \vec{k}', \lambda' | T^{(2)}(E) | 1; \vec{k}, \lambda \rangle = \langle 1; \vec{k}', \lambda' | V \frac{1}{E - H_0 + i\epsilon} V | 1; \vec{k}, \lambda \rangle$$

$$= \sum_N \frac{\langle 1; \vec{k}', \lambda' | V | N; 0 \rangle \langle N; 0 | V | 1; \vec{k}, \lambda \rangle}{E - E_N + i\epsilon}. \quad (72)$$

Here we note that we will take $E = E_F = E_1 + \omega(\vec{k}')$, which is also $E = E_1 + \omega(\vec{k})$. We sum over all atom states $N$. Since (by our choice of photon energy) we will want $E$ to be very close to $E_2$, the dominant contribution is from $N = 2$. Thus (when $E$ is close to $E_2$)

$$\langle 1; \vec{k}', \lambda' | T^{(2)}(E) | 1; \vec{k}, \lambda \rangle \approx \frac{\langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle}{E - E_2 + i\epsilon}. \quad (73)$$

That's a pretty answer, but it is a little suspicious: this is perturbation theory, so we are supposed to get a small answer, but our answer is big because of the small denominator.

If we go to higher orders of perturbation theory, do we get more factors of our small denominator? Yes. At order 4 we have

$$\langle 1; \vec{k}', \lambda' | T^{(4)}(E) | 1; \vec{k}, \lambda \rangle \approx \langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \frac{1}{E - E_2 + i\epsilon}$$

$$\times \langle 2; 0 | V \frac{1}{E - H_0 + i\epsilon} V | 2; 0 \rangle \frac{1}{E - E_2 + i\epsilon} \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle. \quad (74)$$

This has two factors of the small denominator, so it is not a tiny additional term. At order 6 we have

$$\langle 1; \vec{k}', \lambda' | T^{(6)}(E) | 1; \vec{k}, \lambda \rangle \approx \langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \frac{1}{E - E_2 + i\epsilon}$$

$$\times \langle 2; 0 | V \frac{1}{E - H_0 + i\epsilon} V | 2; 0 \rangle \frac{1}{E - E_2 + i\epsilon} \times \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle. \quad (75)$$
At order $2 + 2n$ we have
\[
\langle 1; \vec{k}', \lambda' | \mathcal{T}^{(2+2n)}(E) | 1; \vec{k}, \lambda \rangle \approx \frac{\langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle}{E - E_2 + i\epsilon} \times \left( \frac{X}{E - E_2 + i\epsilon} \right)^n .
\] (76)

where
\[
X = \langle 2; 0 | V \frac{1}{E - H_0 + i\epsilon} V | 2; 0 \rangle .
\] (77)

Now $X$ has two factors of $V$ so it is small, but for each $X$ there is one factor of the small denominator, so the ratio could be large, depending on how small the denominator is.

Clearly what we should do is add up the contributions that have the potential not to be small:
\[
\langle 1; \vec{k}', \lambda' | \mathcal{T}(E) | 1; \vec{k}, \lambda \rangle \approx \langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle \frac{E - (E_2 + X) + i\epsilon}{E - E_2 + i\epsilon} .
\] (79)

This simplifies to
\[
\langle 1; \vec{k}', \lambda' | \mathcal{T}(E) | 1; \vec{k}, \lambda \rangle \approx \frac{\langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle}{E - (E_2 + X) + i\epsilon} .
\] (80)

That’s amazing. The net effect of the interactions is to change the energy of state 2 to $E_2 + X$.

We should find out more about what $X$ is. Since our interaction $V$ creates a photon, we have
\[
X = \sum_N \int d\vec{l} \sum_\lambda \frac{\langle 2; 0 | V | N; l, \lambda \rangle \langle N; l, \lambda | V | 2; 0 \rangle}{E - E_N - \omega(l) + i\epsilon} .
\] (81)
Any atom state $N$ with $E_N < E_2$ and $\langle N; l, \lambda | V | 2; 0 \rangle \neq 0$ can contribute. Certainly state 1 works. Let’s assume it is the only one. Then

$$X = \int d\vec{l} \sum_{\lambda} \frac{|\langle 1; l, \lambda | V | 2; 0 \rangle|^2}{E - E_1 - \omega(\vec{l}) + i\epsilon} . \quad (82)$$

We analyzed this in our analysis of decaying states in the notes on time dependent perturbation theory. Recall that we can write

$$\frac{1}{E - E_1 - \omega(\vec{l}) + i\epsilon} = \frac{1}{[E - E_1 - \omega(\vec{l})]_P} - i\pi\delta(E - E_1 - \omega(\vec{l})) , \quad (83)$$

where $[\cdots]_P$ denotes a principle value prescription when integrating over the singularity. Thus

$$X = \Delta - i\Gamma/2 , \quad (84)$$

where

$$\Delta = \sum_{\lambda} \int d\vec{l} \frac{|\langle 1; l, \lambda | V | 2; 0 \rangle|^2}{[E - E_1 - \omega(\vec{l})]_P} ,$$

$$\Gamma = \sum_{\lambda} \int d\vec{l} 2\pi\delta(E - E_1 - \omega(\vec{l})) |\langle 1; l, \lambda | V | 2; 0 \rangle|^2 . \quad (85)$$

In simple examples, one can perform the integrals to calculate $\Delta$ and $\Gamma$. The dipole approximation can be helpful for this purpose. The values of $\Delta$ and $\Gamma$ depend on $E$. In our application, we are interested in these values for $E \approx E_2$. Thus we use $\Delta(E) \rightarrow \Delta(E_2)$ and $\Gamma(E) \rightarrow \Gamma(E_2)$

Let us now state the result again, evaluating $E$ at its physical value $E = E_1 + \omega(\vec{k}') = E_1 + \omega(\vec{k})$:

$$\langle 1; \vec{k}', \lambda' | T(E_F) | 1; \vec{k}, \lambda \rangle \approx \frac{\langle 1; \vec{k}', \lambda' | V | 2; 0 \rangle \langle 2; 0 | V | 1; \vec{k}, \lambda \rangle}{E_1 + \omega(\vec{k}) - (E_2 + \Delta) + i\Gamma/2} . \quad (86)$$

We see that there is a shift $\Delta$ in the energy of state 2. More significantly, the energy of state 2 acquires an imaginary part $-i\Gamma/2$. We recall from our previous analysis $1/\Gamma$ is the lifetime of state 2. That is, state 2 decays with a time dependence $\exp(-\Gamma t)$.

In our imagined scattering experiment, we are not measuring the time that state 2 stays there. If we want to measure times accurately, then we
cannot keep our photon beam on for a long time, so we cannot know the energy of the photons accurately. Here, we assume that the photon energy is very precisely known. Then, even if we tune $\omega(k)$ to make $E_1 + \omega(\vec{k}) - (E_2 + \Delta) = 0$, we do not get an infinite cross section because the pole in the denominator has moved away from the real energy axis. In fact, the cross section is proportional to

$$f = \frac{1}{|E_1 + \omega(\vec{k}) - (E_2 + \Delta) + i\Gamma/2|^2}$$

\[= \frac{1}{(E_1 + \omega(\vec{k}) - (E_2 + \Delta))^2 + \Gamma^2/4}. \tag{87}\]

The relativistic version of this is known as a Breit-Wigner factor. It is a sharply peaked function if $\Gamma$ is small. One then speaks of a “narrow resonance.” We should note that $\Delta$ and $\Gamma$ are functions of $\omega(\vec{k})$. However, for a narrow resonance one can simply evaluate $\Delta$ and $\Gamma$ at $\omega(\vec{k}) = E_2 - E_1$.

We were wondering what state 2 is if it is not really a state because it decays. Now we see that it is a pole in the S-matrix that is off the real energy axis.

9 Relation to bound states

Notice that the transition operator $\mathcal{T}$ obeys

$$\mathcal{T}(E) = V + V \frac{1}{E - H_0 + i\epsilon} \mathcal{T}(E). \tag{88}\]

This is an operator equation that we could imagine solving for $\mathcal{T}$. In fact, if we solve it perturbatively, the solution is Eq. (71).

We can do something else with it. We note that we can consider $\mathcal{T}$ to be a function of a complex variable $E$, with $\mathcal{T}(E)$ defined by

$$\mathcal{T}(E) = V + V \frac{1}{E - H_0} \mathcal{T}(E). \tag{89}\]

Then the “physical” value is obtained by letting $E$ approach a positive value $E_F$ from the upper half $E$ plane. That is, we let $E = E_F + i\epsilon$.

We can take the defining equation and rewrite it as

$$\left[1 - V \frac{1}{E - H_0}\right] \mathcal{T}(E) = V. \tag{90}\]

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Thus

\[
[E - H_0 - V] \frac{1}{E - H_0} T(E) = V ,
\]

so

\[
T(E) = [E - H_0] \frac{1}{E - H} V ,
\]

Here \( H = H_0 + V \) is the full hamiltonian. Take any matrix element of \( T(E) \) and insert a sum over eigenstates \( |n\rangle \) of \( H \):

\[
\langle \phi_2 | T(E) | \phi_1 \rangle = \sum_n \langle \phi_2 | E - H_0 | n \rangle \frac{1}{E - E_n} \langle n | V | \phi_1 \rangle ,
\]

Thus \( \langle \phi_2 | T(E) | \phi_1 \rangle \) has a pole when \( E \) equals any bound state energy \( E_n \) of the full hamiltonian \( H \). That is, if you were to solve exactly for \( T(E) \), then by analytically continuing from the region that you started in you can find the bound state energies for your potential as poles of the scattering amplitude.

The function \( \langle \phi_2 | T(E) | \phi_1 \rangle \) is also non-analytic when \( E \) is in the range of energies of unbound eigenstates of \( H \). However for unbound states the sum over \( n \) is really an integral and we have a continuous singularity, usually called a cut, instead of a pole.

\section{10 The Lippmann-Schwinger equation}

In this and the following sections, we restrict our analysis to the scattering of non-relativistic particles from a potential.

Let us turn Eq. (88) into an equation for a wave function. Define the wave function \( |\psi_\uparrow\rangle \) by

\[
|\psi_\uparrow\rangle = \left[ 1 + \frac{1}{E_F - H_0 + i\epsilon} T \right] |k_1\rangle
\]

so that

\[
V |\psi_\uparrow\rangle = T |k_1\rangle .
\]

(Here the subscript “+” refers to the “+i\epsilon” in the denominator in the equation for \( T \).) With this definition, we have

\[
|\psi_\uparrow\rangle = |k_1\rangle + \frac{1}{E_F - H_0 + i\epsilon} T |k_1\rangle .
\]
That is
\[ |\psi_+\rangle = |\vec{k}_1\rangle + \frac{1}{E_F - H_0 + i\epsilon} V |\psi_+\rangle . \] (97)

This is the Lippmann-Schwinger equation. Notice that if we multiply it by
\[ E_F - H_0 \] and use \[ [E_F - H_0] |\vec{k}_1\rangle = 0, \]
we get
\[ [H_0 + V] |\psi_+\rangle = E_F |\psi_+\rangle . \] (98)

That is, \[ |\psi_+\rangle \] satisfies the time-independent Schrödinger equation. Essentially, the arrangement in the Lippmann-Schwinger equation tells us the boundary conditions.

We can solve the Lippmann-Schwinger equation perturbatively, giving
\[
|\psi_+\rangle = |\vec{k}_1\rangle \\
+ \frac{1}{E_F - H_0 + i\epsilon} V |\vec{k}_1\rangle \\
+ \frac{1}{E_F - H_0 + i\epsilon} V \frac{1}{E_F - H_0 + i\epsilon} V |\vec{k}_1\rangle \\
+ \cdots . \] (99)

Evidently, this is the same as using our perturbative expansion of \( T \).

11 The Green function

The operator \( 1/[E_F - H_0 + i\epsilon] \) obeys
\[ [E_F - H_0] \frac{1}{E_F - H_0 + i\epsilon} = 1 . \] (100)

In a position representation of this operator, \( \langle \vec{x}' | 1/[E_F - H_0 + i\epsilon] | \vec{x} \rangle \) is a Green function for the time independent free particle Schrödinger equation. It obeys
\[
\left[ E_F - \frac{1}{2m} \vec{\nabla}_x^2 \right] \langle \vec{x}' | 1/E_F - H_0 + i\epsilon | \vec{x} \rangle = \delta(\vec{x} - \vec{x}') . \] (101)

The “\(+i\epsilon\)” specifies the boundary conditions.
We can find \( \langle \vec{x} | 1/(E_F - H_0 + i\epsilon) | \vec{x}' \rangle \) by Fourier transforming,
\[
\langle \vec{x} | 1 \rangle \frac{1}{E_F - H_0 + i\epsilon} \langle \vec{x}' \rangle = \int d\vec{k} \langle \vec{x} | \vec{k} \rangle \frac{1}{E_F - \vec{k}^2/(2m) + i\epsilon} \langle \vec{k} | \vec{x}' \rangle = \int \frac{d\vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{x} - \vec{x}')} \frac{1}{E_F - \vec{k}^2/(2m) + i\epsilon}.
\]

(102)

We can perform the integration by using spherical polar coordinates for \( \vec{k} \), with the z-axis chosen in the direction of \( \vec{x} - \vec{x}' \):
\[
\langle \vec{x} | \frac{1}{E_F - H_0 + i\epsilon} | \vec{x}' \rangle = \frac{2m}{(2\pi)^2} \int_0^\infty k^2 dk \frac{1}{k_F^2 - k^2 + i\epsilon} \int_{-1}^1 d\cos \theta e^{ik|\vec{x} - \vec{x}'| \cos \theta} = \frac{m}{(2\pi)^2} \int_{-\infty}^\infty k dk \frac{1}{k_F^2 - k^2 + i\epsilon} \frac{1}{ik|\vec{x} - \vec{x}'|} \left(e^{ik|\vec{x} - \vec{x}'|} - e^{-ik|\vec{x} - \vec{x}'|}\right) \quad \text{ (103)}
\]

Note that in the last line, we got the \( \epsilon \) right: putting the denominator back together we get \( k_F^2 - k^2 + i\epsilon k_F \), which has the right sign for the \( \epsilon \) because \( k_F > 0 \). We can perform the \( k \)-integration by closing the integration contour in either the upper or lower half plane. For the term with \( \exp(ik|\vec{x} - \vec{x}'|) \), we need to close the contour in the upper half \( k \) plane, giving us the residue of the pole at \( k = k_F \). For the term with \( \exp(-ik|\vec{x} - \vec{x}'|) \), we need to close the contour in the lower half \( k \) plane, giving us the residue of the pole at \( k = -k_F \). This gives
\[
\langle \vec{x} | \frac{1}{E_F - H_0 + i\epsilon} | \vec{x}' \rangle = -\frac{m}{2\pi} \frac{1}{|\vec{x} - \vec{x}'|} e^{ik_F|\vec{x} - \vec{x}'|}. \quad \text{ (104)}
\]

If we consider this as a function of \( \vec{x} \), we have a spherical wave centered at \( \vec{x}' \). For large \( |\vec{x} - \vec{x}'| \), it looks like a plane wave. To see this, define
\[
\tilde{k}'_F = \frac{k_F (\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|}. \quad \text{ (105)}
\]
Then
\[ e^{i k_F |\vec{x} - \vec{x}'|} = e^{i \vec{k}'_F \cdot (\vec{x} - \vec{x}')} . \] (106)

If \(|\vec{x} - \vec{x}'| \gg 1/k_F\), then locally (within a region containing a few wavelengths), \(k'_F\) is approximately constant. Then our factor looks like a plane wave with momentum \(k'_F\) that points away from the center of our wave at \(\vec{x} = \vec{x}'\) and has magnitude equal to \(k_F\). Notice that this is an outgoing wave: \(k'_F\) points away from the wave center. This is a consequence of our having a \(+i\epsilon\) in the denominator \(E_F - k^2/(2m) + i\epsilon\).

12 The wave function at large distance

In this section, we examine the behavior of the wave function \(\psi_+ (\vec{x} ) \equiv \langle \vec{x} | \psi_+ \rangle\) for large \(|\vec{x}|\). From Eq. (97), we have

\[ \langle \vec{x} | \psi_+ \rangle = \langle \vec{x} | \vec{k}_I \rangle + \int d\vec{x}' \frac{1}{E_F - H_0 + i\epsilon} \langle \vec{x}' | V(\vec{x}') \rangle \langle \vec{x}' | \psi_+ \rangle . \] (107)

That is

\[ \psi_+ (\vec{x} ) = (2\pi)^{-3/2} e^{i \vec{k}_I \cdot \vec{x}} \]
\[ - \frac{m}{2\pi} \int d\vec{x}' \frac{1}{|\vec{x} - \vec{x}'|} e^{i k_F |\vec{x} - \vec{x}'|} V(\vec{x}') \psi_+ (\vec{x}' ) \] (108)

We are interested in the behavior of \(\psi_+ (\vec{x} )\) for large \(|\vec{x}|\). We assume that \(V(\vec{x}')\) is concentrated in a region of finite, not large, \(|\vec{x}'|\).

Let

\[ \vec{x} = R \bar{n} , \] (109)

where \(R = |\vec{x}|\) and \(\bar{n}\) is a unit vector in the direction of \(\vec{x}\). Let us see what this looks like for fixed \(\bar{n}\) in the limit of large \(R\). In the exponent, we have

\[ k_F |\vec{x} - \vec{x}'| = k_F R \left| \bar{n} - \frac{\vec{x}'}{R} \right| \]
\[ = k_F R \left[ 1 - 2 \bar{n} \cdot \vec{x}' + \frac{(\vec{x}')^2}{R^2} \right]^{1/2} \] (110)
\[ = k_F R - k_F \bar{n} \cdot \vec{x}' + O(1/R) . \]
We can take the limit $R \to \infty$ and throw away the term proportional to $1/R$ or higher powers of $1/R$, but we need to keep the term in the exponent with no powers of $R$. In the denominator, we can simply write

$$\frac{1}{|\vec{x} - \vec{x}'|} = \frac{1}{R} \left[ 1 + O\left( \frac{1}{R} \right) \right]$$

and drop the terms that are suppressed by powers of $1/R$. This gives

$$\psi_+(\vec{x}) \sim (2\pi)^{-3/2} e^{i\vec{k}_1 \cdot \vec{x}}$$

$$- \frac{m}{2\pi} \frac{1}{R} e^{ik_F R} \int d\vec{x}' e^{-ik_F \vec{n} \cdot \vec{x}'} V(\vec{x}') \psi_+(\vec{x}') \ .$$

Now note that

$$\int d\vec{x}' e^{-ik_F \vec{n} \cdot \vec{x}'} V(\vec{x}') \psi_+(\vec{x}') = (2\pi)^{3/2} \langle k_F \vec{n} | T | \vec{k}_1 \rangle \ .$$

Thus for large $R$ we have

$$\psi_+(R\vec{n}) \sim (2\pi)^{-3/2} \left[ e^{i\vec{k}_1 \cdot \vec{n} R} - \frac{1}{R} e^{ik_F R} (2\pi)^2 m \langle k_F \vec{n} | T | \vec{k}_1 \rangle \right] \ .$$

We can also write this as

$$\psi_+(R\vec{n}) \sim (2\pi)^{-3/2} \left[ e^{i\vec{k}_1 \cdot \vec{n} R} + \frac{1}{R} e^{ik_F R} f(k_F \vec{n}, \vec{k}_1) \right] \ .$$

where

$$f(k_F \vec{n}, \vec{k}_1) \equiv -(2\pi)^2 m \langle k_F \vec{n} | T | \vec{k}_1 \rangle \ .$$

There is an overall normalization factor $(2\pi)^{-3/2}$. There is a plane wave that represents the incoming particle, $\exp(i\vec{k}_1 \cdot \vec{x})$. Then there is an outgoing wave factor $\exp(ik_F R)$ times $1/R$. The coefficient of this is $f(k_F \vec{n}, \vec{k}_1)$, which is proportional to the transition matrix element for scattering the incoming
momentum eigenstate $|\vec{k}_1\rangle$ to an outgoing momentum eigenstate $\langle k_F\vec{n}|$. Also note that the differential cross section $d\sigma/d\Omega_F$, as given in Eq. (59), is

$$\frac{d\sigma}{d\Omega_F} = |f(k_F\vec{n}, \vec{k}_1)|^2. \quad (118)$$

If we want to find the scattering amplitude $\langle k_F\vec{n}|T|\vec{k}_1\rangle$ and thus the cross section, we now have two choices. We can use our perturbation theory, for which the first order approximation is

$$\langle k_F\vec{n}|T|\vec{k}_1\rangle \sim \langle k_F\vec{n}|V|\vec{k}_1\rangle. \quad (119)$$

Alternatively, we can solve the Lippmann-Schwinger equation for $\psi_+(\vec{x})$ and pick out the behavior of this function at large $|\vec{x}|$. The limiting form of this function depends on the direction of $\vec{x}$. The coefficient of $\exp(ik_FR)/R$ gives the scattering amplitude.

We can also understand the relation of the cross section to $f(k_F\vec{n}, \vec{k}_1)$ in a direct way based on wave functions. We have a plane wave coming in and, far away from the scattering center, almost a plane wave going out. The ratio of the number of particles that cross an area $dA$ in some fixed time interval in the two waves is the ratio of the squares of the coefficients of the two plane wave factors:

$$\frac{dN_F}{dN_1} \frac{dA}{dA} = \frac{1}{R^2} |f(k_F\vec{n}, \vec{k}_1)|^2. \quad (120)$$

Far away from the scattering center, an area $dA$ subtends a solid angle $d\Omega_F = dA/R^2$. Thus the ratio of the number of particles per unit solid angle in the outgoing wave to the number of particles per unit area in the incoming wave is

$$\frac{dN_F}{dN_1} \frac{d\Omega_F}{d\Omega_1} = |f(k_F\vec{n}, \vec{k}_1)|^2. \quad (121)$$

This ratio is just what we mean by the differential cross section. Thus

$$\frac{d\sigma}{d\Omega_F} = |f(k_F\vec{n}, \vec{k}_1)|^2. \quad (122)$$

### 13 The optical theorem

There is a relation, known as the optical theorem, between the scattering amplitude for forward scattering and the total cross section. This relation is
derived from the fact that the scattering operator $S$ is unitary. The derivation is simple in outline:

\[
1 = S^\dagger S \\
= [1 + ic\, T^\dagger][1 - ic\, T] \\
= 1 + ic\, [T^\dagger - T] + c^2\, T^\dagger T
\]  

so

\[
-i[T^\dagger - T] = c\, T^\dagger T.  
\]  

(124)

When this relation is taken between \(\langle \vec{k}_1 | \cdots | \vec{k}_1 \rangle\), the left hand side is proportional to the imaginary part of the forward scattering amplitude and the right hand side is the total cross section. However, we have to be careful because the “c” here is a delta function. Let us, therefore, try a careful derivation.

Let’s look back at the $S$ matrix, Eq. (47),

\[
\langle \vec{k}_F | S | \vec{k}_I \rangle = \langle \vec{k}_F | \vec{k}_1 \rangle + 2\pi\delta(E_F - E_I)(-i)\langle \vec{k}_F | T | \vec{k}_1 \rangle.  
\]

(125)

Consider also the complex conjugate of this with a state $|\vec{k}_1'\rangle$ that is slightly different from $|\vec{k}_1\rangle$,

\[
\langle \vec{k}_1'| S^\dagger | \vec{k}_F \rangle = \langle \vec{k}_1'| \vec{k}_F \rangle + 2\pi\delta(E_F - E_I')(+i)\langle \vec{k}_F | T | \vec{k}_1' \rangle^*.  
\]

(126)

Multiply these together and integrate over $\vec{k}_F$:

\[
\int d\vec{k}_F \langle \vec{k}_1'| S^\dagger | \vec{k}_F \rangle \langle \vec{k}_F | S | \vec{k}_1 \rangle \\
= \int d\vec{k}_F \langle \vec{k}_1'| \vec{k}_F \rangle \langle \vec{k}_F | \vec{k}_1 \rangle \\
- i \int d\vec{k}_F 2\pi\delta(E_F - E_I)\langle \vec{k}_1'| \vec{k}_F \rangle \langle \vec{k}_F | T | \vec{k}_1 \rangle \\
+ i \int d\vec{k}_F 2\pi\delta(E_F - E_I')\langle \vec{k}_F | \vec{k}_1 \rangle \langle \vec{k}_F | T | \vec{k}_1' \rangle^* \\
+ \int d\vec{k}_F 2\pi\delta(E_F - E_I')2\pi\delta(E_F - E_I)\langle \vec{k}_F | T | \vec{k}_1 \rangle \langle \vec{k}_F | T | \vec{k}_1' \rangle^*.  
\]

(127)

If we recognize that $\langle \vec{k}_F | \vec{k}_1 \rangle$ is a delta function and that the integral of
\[ |\vec{k}_F\rangle\langle \vec{k}_F| \] is the unit operator, we have
\[
\langle \vec{k}'_1| S^\dagger S| \vec{k}_1 \rangle = \langle \vec{k}'_1| \vec{k}_1 \rangle - i2\pi\delta(E'_1 - E_1)\langle \vec{k}'_1| T| \vec{k}_1 \rangle + i2\pi\delta(E'_1 - E_1)\langle \vec{k}_1| T| \vec{k}'_1 \rangle^* + 2\pi\delta(E'_1 - E_1) \int d\vec{k}_F \ 2\pi\delta(E_F - E_1)\langle \vec{k}_F| T| \vec{k}_1 \rangle \langle \vec{k}_F| T| \vec{k}'_1 \rangle^* .
\] (128)

So far we have simply written \( S \) as a matrix in the momentum representation and multiplied \( S^\dagger \) by \( S \). Now we insert an important condition that follows directly from the definition of \( S \):

\[
S^\dagger S = 1 .
\] (129)

That is, \( S \) is unitary. This gives
\[
\langle \vec{k}'_1| \vec{k}_1 \rangle = \langle \vec{k}'_1| \vec{k}_1 \rangle - i2\pi\delta(E'_1 - E_1)\langle \vec{k}'_1| T| \vec{k}_1 \rangle + i2\pi\delta(E'_1 - E_1)\langle \vec{k}_1| T| \vec{k}'_1 \rangle^* + 2\pi\delta(E'_1 - E_1) \int d\vec{k}_F \ 2\pi\delta(E_F - E_1)\langle \vec{k}_F| T| \vec{k}_1 \rangle \langle \vec{k}_F| T| \vec{k}'_1 \rangle^* .
\] (130)

We can cancel the two \( \langle \vec{k}'_1| \vec{k}_1 \rangle \) terms and then take the coefficient of \( 2\pi\delta(E'_1 - E_1) \):
\[
0 = -i\langle \vec{k}'_1| T| \vec{k}_1 \rangle + i\langle \vec{k}_1| T| \vec{k}'_1 \rangle^* + \int d\vec{k}_F \ 2\pi\delta(E_F - E_1)\langle \vec{k}_F| T| \vec{k}_1 \rangle \langle \vec{k}_F| T| \vec{k}'_1 \rangle^* .
\] (131)

We have been careful to keep \( \vec{k}'_1 \) just a little different from \( \vec{k}_1 \), but now we can take the limit in which they are equal:
\[
i\langle \vec{k}'_1| T| \vec{k}_1 \rangle - i\langle \vec{k}_1| T| \vec{k}'_1 \rangle^* = \int d\vec{k}_F \ 2\pi\delta(E_F - E_1)\langle \vec{k}_F| T| \vec{k}_1 \rangle \langle \vec{k}_F| T| \vec{k}'_1 \rangle^* .
\] (132)
The left hand side is minus two times the imaginary part of $\langle \vec{k}_I | T | \vec{k}_I \rangle$. By using

$$\int d\vec{k} \cdots = \int m k dE \ d\Omega \cdots ,$$  \hspace{1cm} (133)

we can eliminate the energy conserving delta function on the right hand side. This gives

$$-2 \text{Im}\langle \vec{k}_I | T | \vec{k}_I \rangle = 2\pi m k_F \int d\Omega_F |\langle \vec{k}_F | T | \vec{k}_I \rangle|^2 .$$  \hspace{1cm} (134)

Recall from Eq. (59) that

$$|\langle \vec{k}_F | T | \vec{k}_I \rangle|^2 = \frac{1}{(2\pi)^4 m^2} \frac{d\sigma}{d\Omega_F} .$$  \hspace{1cm} (135)

Thus

$$-\text{Im}\langle \vec{k}_I | T | \vec{k}_I \rangle = \frac{k_I}{2m(2\pi)^3} \int d\Omega_F \frac{d\sigma}{d\Omega_F} .$$  \hspace{1cm} (136)

We call the integral of $d\sigma/d\Omega_F$ the total cross section, $\sigma_T$. Thus

$$-\text{Im}\langle \vec{k}_I | T | \vec{k}_I \rangle = \frac{k_I}{2m(2\pi)^3} \sigma_T .$$  \hspace{1cm} (137)

This says that the imaginary part of the forward scattering amplitude is proportional to the total cross section. The proportionality constant depends on what we mean by “forward scattering amplitude.” If we use Eq. (117),

$$\langle \vec{k}_F | T | \vec{k}_I \rangle = \frac{1}{(2\pi)^2 m} f(\vec{k}_F, \vec{k}_I) ,$$  \hspace{1cm} (138)

we obtain

$$\text{Im} f(\vec{k}_I, \vec{k}_I) = \frac{k_I}{4\pi} \sigma_T .$$  \hspace{1cm} (139)

### 14 The eikonal approximation

There is an approximation that is useful for small angle scattering of a highly energetic incoming particle from a smooth potential. We consider the case
that the incoming momentum $k_1$ is large and the potential is smooth: if $d$ is
the distance range over which the potential varies significantly, then $k_1d \ll 1$.

In addition, the potential should be sufficiently strong to actually scatter
the particle. To see what this means, consider a semiclassical approximation
for the phase accumulated by a particle moving through the potential along a
straight line along the $z$-axis at transverse position $b$, starting at $z$-coordinate $z_0$ and ending at $z$:

$$
\phi(b, z, z_0) = \int_{z_0}^{z} dz' \ k(z', b)
= \int_{z_0}^{z} dz' \ \sqrt{k_1^2 - 2mV(z', b)}
\approx \int_{z_0}^{z} dz' \ \left\{ k_1 - \frac{m}{k_1} V(z', b) \right\}
= k_1(z - z_0) - \frac{m}{k_1} \int_{z_0}^{z} dz' \ V(z', b). \tag{140}
$$

There is a term $k_1(z - z_0)$ that gives the phase of a plane wave. This phase
is present even when $V$ is not there. Then the potential produces an extra
phase. For $z_0 \to -\infty$ and $z \to \infty$, the extra phase is

$$
\Delta \phi(b) = -\frac{m}{k_1} \int_{-\infty}^{\infty} dz' \ V(z', b). \tag{141}
$$

We are interested in the case that $V$ is strong enough that $\Delta \phi(b)$ is not
negligible.

Let us see how this phase gets into the wave function if we use a large $k_1$
approximation. Let

$$
\psi_+(z, b) = (2\pi)^{-3/2} e^{ik_1 z} \Phi(z, b) \tag{142}
$$

where, we suppose, $\Phi(z, b)$ is slowly varying (compared to the fast variation
of $\exp(ik_1 z)$). The wave function $\psi_+(z, b)$ obeys

$$
\left[ -\frac{1}{2m} \frac{\partial^2}{\partial z^2} - \frac{1}{2m} \nabla_b^2 + V(z, b) - \frac{k_1^2}{2m} \right] \psi_+(z, b) = 0. \tag{143}
$$

As an equation for $\Phi$, this becomes

$$
\left[ -ik_1 \frac{\partial}{m \partial z} - \frac{1}{2m} \frac{\partial^2}{\partial z^2} - \frac{1}{2m} \nabla_b^2 + V(z, b) \right] \Phi(z, b) = 0. \tag{144}
$$
This is without approximation. If we now say that $\Phi$ is slowly varying, we can neglect the derivatives of $\Phi$ except for the one that is multiplied by $k_1$. Then
\[ \left[ -i \frac{k_1}{m} \frac{\partial}{\partial z} + V(z, b) \right] \Phi(z, b) \approx 0 \quad (145) \]

The solution of this equation is
\[ \Phi(z, b) \approx \exp \left( -i \frac{m}{k_1} \int_{-\infty}^{z} dz' \ V(z', b) \right) \quad (146) \]

This solution obeys the boundary condition $\Phi(z, b) \rightarrow 1$ for $z \rightarrow -\infty$, so that $(2\pi)^{-3/2} \exp(i k_1 z) \Phi(z, b)$ approaches the desired incoming plane wave for large negative $z$. With this solution for $\Phi$, we have
\[ \psi_+(z, b) \approx (2\pi)^{-3/2} e^{ik_1 z} \exp \left( -i \frac{m}{k_1} \int_{-\infty}^{z} dz' \ V(z', b) \right) \quad (147) \]

We can turn this approximation for $\psi_+(x)$ into an approximation for the scattering amplitude by using
\[ f(\vec{k}_F, \vec{k}_1) = - (2\pi)^2 m \left\langle \vec{k}_F | T | \vec{k}_1 \right\rangle \\
= - (2\pi)^2 m \left\langle \vec{k}_F | V | \psi_+ \right\rangle \quad (148) \]

We take $\vec{k}_1$ along the $z$-axis and we let $\vec{k}_F$ have a transverse component $\vec{k}_\perp$ that is much smaller than its $z$-component, corresponding to small angle scattering. The size of the $z$-component of $\vec{k}_F$ is $|k_1^2 - k_\perp^2|^{1/2}$, but we can approximate this by just $k_1$. Thus
\[ \vec{k}_F \approx k_1 \hat{z} + \vec{k}_\perp \quad (149) \]
Then
\[ f(\vec{k}_F, \vec{k}_I) = -\frac{m}{2\pi} \int dz \int db \ e^{-ik_Iz - ik_\perp \cdot b} V(z, b) \]
\[ \times e^{ik_Iz} \exp \left( -i \frac{m}{k_1} \int dz' \ V(z', b) \right) \]
\[ = -\frac{m}{2\pi} \int db \ e^{-ik_\perp \cdot b} \]
\[ \times \int dz \ V(z, b) \exp \left( -i \frac{m}{k_1} \int dz' \ V(z', b) \right) \]
\[ = -\frac{m}{2\pi} \int db \ e^{-ik_\perp \cdot b} \left( i \frac{k_1}{m} \right) \int dz \ \frac{d}{dz} \exp \left( -i \frac{m}{k_1} \int dz' \ V(z', b) \right) \]
\[ (150) \]

Performing the \(z\)-integration gives
\[ f(\vec{k}_F, \vec{k}_I) = -\frac{ik_1}{2\pi} \int db \ e^{-ik_\perp \cdot b} \left[ \exp \left( -i \frac{m}{k_1} \int dz' \ V(z', b) \right) - 1 \right]. \quad (151) \]

This is the eikonal approximation to the scattering amplitude. It has a simple interpretation. There is an incoming plane wave. The plane wave represents particles that travel through the potential on straight line paths; the paths are not deflected because the momentum of the particles is so high. However, the particles accumulate a \(b\) dependent phase factor as they pass through the potential. This means that they acquire a little bit of transverse momentum. We find the amplitude in transverse momentum space by Fourier transforming from transverse position to transverse momentum. That gives the scattering amplitude. Our wave function includes the incoming plane wave, but this is subtracted before we perform the Fourier transform. With the “1” subtracted, the quantity that we are Fourier transforming vanishes for large \(|b|\).

**Exercise 14.1** We can think of the eikonal approximation problem in a different way that is very similar to classical optics problems that you are familiar with. The incoming wave is distorted by the potential, acquiring an extra phase factor. We can calculate this phase factor in the semiclassical approximation that we used above. Then at a position \(z_1\) that is large enough to be
outside the range of the potential but not larger than that, the wave function is
\[ \psi_+(z_1, b') \approx (2\pi)^{-3/2} e^{i k_1 z_1} \exp \left( -i \frac{m}{k_1} \int_{-\infty}^{\infty} dz' V(z', b') \right). \] (152)

Now we would like to know the wave function at a particle detector that is far away from the scattering center at a position \((z, z_\theta)\) where \(\theta\) is a vector in the two transverse dimensions, with \(|\theta| \ll 1\). For the propagation from \((z_1, b')\) to \((z, z_\theta)\), one can use Eq. (144) as an approximation, but we cannot neglect the \(-\nabla_\theta^2/(2m)\) term because this term can have a big effect if it is applied for propagation over a very big distance. However, the propagation is simple because for \(z > z_1\) the potential vanishes.

Solve Eq. (144) with \(V = 0\) to find \(\psi_+(z, z_\theta)\) in terms of \(\psi_+\) at fixed \(z\)-coordinate equal to \(z_1\). This is similar to problems that we have done before and it is similar to problems in optics. Use your solution and the form Eq. (116) to pick out the scattering amplitude \(f(k_1 \hat{z}, k_1 \theta)\).

What you see from this exercise is that the scattering amplitude far from the scattering center is analogous to the diffraction pattern formed at a screen far from the scattering center in an optics experiment in which an incoming electromagnetic wave is distorted by some sort of scattering. (Letting it go through two slits is the simplest example.)

15 Partial waves

For many purposes, particularly in connection with scattering of low energy particles from a spherically symmetric potential, it is useful to use an angular momentum basis.

We first need to translate between plane waves and angular momentum eigenstates. Let the states \(|\vec{k}\rangle\) denote plane wave states, eigenstates of \(p_x, p_y, p_z\). Let us find a basis for the quantum Hilbert space consisting of states
\[ |E, l, m\rangle \] (153)
that are eigenstates of \(\vec{p}^2/(2m), \vec{L}^2,\) and \(L_z\). We will normalize these to
\[ \langle E', l', m'|E, l, m\rangle = \delta(E' - E) \delta_{l l'} \delta_{m m'} \] (154)
The translation between these is given by

$$\langle \vec{k} | E, l, m \rangle = \frac{1}{\sqrt{mk}} \delta \left( \frac{\vec{k}^2}{2m} - E \right) Y_l^m(\hat{k}) ,$$

(155)

where \( \hat{k} \) is a unit vector in the direction of \( \vec{k} \). Our book makes this seem difficult. However, the \( Y_l^m \) factor is obvious, given our extensive knowledge of angular momentum. Similarly, the delta function is obvious. The only thing that needs checking is the normalization:

$$\langle E', l', m' | E, l, m \rangle = \frac{1}{mk} \int d\vec{k} \delta \left( \frac{\vec{k}^2}{2m} - E' \right) \delta \left( \frac{\vec{k}^2}{2m} - E \right) Y_{l'}^{m'}(\hat{k}) Y_l^m(\hat{k})$$

$$= \frac{1}{mk} \int_0^\infty mk d\left( \frac{k^2}{2m} \right) \delta \left( \frac{k^2}{2m} - E' \right) \delta \left( \frac{k^2}{2m} - E \right)$$

$$\times \int d\Omega Y_{l'}^{m'}(\hat{k}) Y_l^m(\hat{k})$$

$$= \delta(E' - E) \delta_{l'l} \delta_{m'm} .$$

(156)

For a plane wave \( \langle \vec{k}_I | \) in the \( z \)-direction, Eq. (155) takes the simple form

$$\langle \vec{k}_I | E, l, m \rangle = \frac{1}{\sqrt{mk_I}} \delta \left( \frac{\vec{k}_I^2}{2m} - E \right) \sqrt{\frac{2l + 1}{4\pi}} \delta_{m,0} .$$

(157)

For a plane wave \( \langle \vec{k}_F | \) in any direction, but for \( m = 0 \), Eq. (155) takes the simple form

$$\langle \vec{k}_F | E, l, 0 \rangle = \frac{1}{\sqrt{mk_F}} \delta \left( \frac{\vec{k}_F^2}{2m} - E \right) \sqrt{\frac{2l + 1}{4\pi}} P_l(\cos \theta_F) .$$

(158)

The position space version of Eq. (155) is

$$\langle \vec{x} | E, l, m \rangle = i^l \sqrt{\frac{2mk}{\pi^l}} j_l(k|\vec{x}|) Y_l^m(\hat{x}) ,$$

(159)

where \( \hat{x} \) is a unit vector in the direction of \( \vec{k} \) and \( j_l(k|\vec{x}|) \) is a spherical Bessel function. Again, the \( Y_l^m \) factor is obvious. The spherical Bessel function is
there because it is the solution of the radial wave function for a free particle with angular momentum \( l \) – provided that we demand that the solution not be singular at \( r = 0 \). To get the factor \( i^l \) and the normalization, you need a real calculation, which I omit.

I will assume that spherical Bessel functions are known from a mathematical physics course or an electrodynamics course. Some information about them is given in Appendix B of Sakurai. One particularly useful relation is the partial wave expansion of a plane wave in the \( z \)-direction,

\[
e^{ikz} = e^{ikr \cos \theta} \sum_l (2l + 1) P_l(\cos \theta) i^l j_l(kr) .
\]  

(160)

We now consider scattering from a spherically symmetric potential. Let’s use the angular momentum decomposition to write the scattering amplitude \( f \),

\[
f(\vec{k}_F, \vec{k}_I) = - (2\pi)^2 m \langle \vec{k}_F \mid T \mid \vec{k}_I \rangle \\
= - (2\pi)^2 m \sum_{l,m} \int dE' \sum_{l',m'} \int dE \\
\times \langle \vec{k}_F \mid E', l', m' \rangle \langle E', l', m' \mid T \mid E, l, m \rangle \langle E, l, m \mid \vec{k}_I \rangle .
\]  

(161)

Since the initial plane wave is in the \( z \)-direction, only \( m = 0 \) contributes. Since the potential is invariant under rotations, the \( L_z \) eigenvalue can’t change, so only \( m' = 0 \) contributes. Also, since the potential is invariant under rotations, the only \( l' \) value that contributes is \( l' = l \). Also, the matrix elements \( \langle \vec{k}_F \mid E', l', m' \rangle \) and \( \langle E, l, m \mid \vec{k}_I \rangle \) contain delta functions that eliminate the integrations over \( E \) and \( E' \). Thus

\[
f(\vec{k}_F, \vec{k}_I) = - \frac{\pi}{k_F} \sum_l (2l + 1) P_l(\cos \theta_F) \langle E_l, l, 0 \mid T \mid E_l, l, 0 \rangle .
\]  

(162)

One often defines the “partial wave amplitude” \( f_l(k) \) by

\[
f_l(k) = - \frac{\pi}{k} \langle E, l, 0 \mid T \mid E, l, 0 \rangle .
\]  

(163)

Then

\[
f(\vec{k}_F, \vec{k}_I) = \sum_l (2l + 1) P_l(\cos \theta_F) f_l(k) .
\]  

(164)
This “partial wave expansion” is particularly useful when only one or a few partial waves are important.

Exercise 15.1 Using partial waves, consider the perturbative expansion for scattering from a spherically symmetric potential. Using the Born approximation, express $f_l(k_I)$ as an integral over position $r$ of $V(r)$ times some other functions. What is this for $l = 0$ and $l = 1$? Which is bigger if $k_I$ is very small?

Exercise 15.2 Consider a particle of mass $m$ that is elastically scattered according to non-relativistic quantum mechanics by a Gaussian potential in three dimensions,

$$V(\vec{r}) = -V_0 e^{-\vec{r}^2/a^2}. \quad (165)$$

Here $V_0 > 0$ and $a$ is a parameter with dimension of length. The incoming particle has wavevector $\vec{k}$ and, after the scattering, the outgoing particle has wavevector $\vec{k}'$. Define $\vec{q} = \vec{k}' - \vec{k}$ and denote the scattering angle by $\theta$.

(a) Show that $|\vec{q}| = 2|\vec{k}| \sin(\theta/2)$.

(b) Using the Born approximation, calculate the scattering amplitude $f(\vec{k}_F, \vec{k}_I)$.

(c) Using your approximate $f(\vec{k}_F, \vec{k}_I)$, calculate the differential scattering cross section $d\sigma/d\Omega$.

(d) Making use of this result, calculate the total scattering cross section $\sigma_T$.

(e) Using your approximate scattering amplitude $f(\vec{k}_F, \vec{k}_I)$, find $f_l(k_I)$ for $l = 0, 1, 2$. 
16 Unitarity and the phase shift

We consider scattering from a spherically symmetric potential. Start with
\begin{equation}
\langle k_F | S | k_i \rangle = \langle k_F | k_i \rangle + 2\pi \delta(E_F - E_i)(-i)\langle k_F | T(E_F) | k_i \rangle .
\end{equation}
(166)
We can think of this as an operator equation,
\[ S = 1 - i \int_{-\infty}^{+\infty} dt \ e^{iH_0 t} T(E_F) e^{-iH_0 t} . \]
(167)
Between energy eigenstates, this gives back Eq. (166). Now we can take matrix elements of this operator equation between states \( \langle E_F, l_F, m_F | \) and \( | E_i, l_i, m_i \rangle \). This gives
\begin{equation}
\langle E_F, l_F, m_F | S | E_i, l_i, m_i \rangle \\
= \langle E_F, l_F, m_F | E_i, l_i, m_i \rangle + 2\pi \delta(E_F - E_i)(-i)\langle E_F, l_F, m_F | T(E_F) | E_i, l_i, m_i \rangle .
\end{equation}
(168)
For the two terms on the right hand side of Eq. (168), we have
\begin{align}
\langle E_F, l_F, m_F | E_i, l_i, m_i \rangle &= \delta(E_F - E_i) \delta_{l_F,l_i} \delta_{m_F,m_i} , \\
\langle E_F, l_F, m_F | T(E_F) | E_i, l_i, m_i \rangle &= \delta_{l_F,l_i} \delta_{m_F,m_i} \langle E_F, l_i, 0 | T(E_F) | E_i, l_i, 0 \rangle .
\end{align}
(169)
Here we have noted that \( T(E_F) \) commutes with \( \vec{L} \), so the matrix element of \( T(E_F) \) vanishes unless \( l_F = l_i \) and \( m_F = m_i \). Also, the matrix element must be independent of \( m_i \), as one can prove by using the fact that the angular momentum raising and lowering operators \( L_\pm \) commute with \( T(E_F) \); thus we can evaluate the matrix element with \( m_F = m_i = 0 \). On the left hand side of Eq. (168), \( S \) commutes with \( H_0 \) and \( \vec{L} \), so \( | E_i, l_i, m_i \rangle \) must be an eigenstate of \( S \). Furthermore, the eigenvalue must be independent of \( m_i \). Call the eigenvalue \( S_i(k_f) \). Then
\begin{equation}
\langle E_F, l_F, m_F | S | E_i, l_i, m_i \rangle = S_i(k_f) \langle E_F, l_F, m_F | E_i, l_i, m_i \rangle \\
= S_i(k_f) \delta(E_F - E_i) \delta_{l_F,l_i} \delta_{m_F,m_i} .
\end{equation}
(170)
These results give
\begin{equation}
S_i(k_f) \delta(E_F - E_i) \delta_{l_F,l_i} \delta_{m_F,m_i} \\
= \delta(E_F - E_i) \delta_{l_F,l_i} \delta_{m_F,m_i} \\
+ 2\pi \delta(E_F - E_i)(-i)\delta_{l_F,l_i} \delta_{m_F,m_i} \langle E_F, l_i, 0 | T(E_F) | E_i, l_i, 0 \rangle .
\end{equation}
(171)
We can cancel the $\delta(E_F - E_1)$ and the $\delta_{l_F,l_I} \delta_{m_F,m_I}$ and also use Eq. (163) to write the matrix element of $T$ in terms of $f_l(k)$. This gives

$$S_l(k) = 1 + 2i k f_l(k) \ . \tag{172}$$

Now since $S$ is a unitary operator, its eigenvalue must be a phase factor. One calls the phase factor $\exp(2i\delta_l(k))$, where $\delta_l$ is the phase shift for the $l$th partial wave. Thus

$$e^{2i\delta_l(k)} = 1 + 2i k f_l(k) \ . \tag{173}$$

We can solve this for $f_l(k)$:

$$f_l(k) = \frac{1}{2ik} \left[ e^{2i\delta_l(k)} - 1 \right] \ . \tag{174}$$

17 The wave function

Let us now look at the wave function. We assume that the potential is spherically symmetric, so that it is a function $V(r)$ of $r = |\vec{x}|$. We shorten $k_I$ and $k_F$ to just $k$. Similarly, we denote the scattering angle $\theta_F$ by just $\theta$. The wave function $\psi_+(\vec{x})$ obeys the Schrödinger equation with energy $E = k^2/(2m)$. For our application, the wave function is independent of the azimuthal angle $\phi$, but it depends on $r$ and $\theta$. We can decompose it in partial waves as

$$(2\pi)^{3/2} \psi_+(\vec{x}) = \sum_{l=0}^{\infty} \frac{l}{2} (2l + 1) P_l(\cos \theta) \psi_l(r) \ . \tag{175}$$

The normalizing factors here are chosen to make the final results simple. Then $\psi_l(r)$ must be a solution of the radial Schrödinger equation

$$\left[ \frac{1}{r} \frac{d^2}{dr^2} r + k^2 - 2m V(r) - \frac{l(l+1)}{r^2} \right] \psi_l(r) = 0 \ . \tag{176}$$

Generally there will be two independent solutions of this equation, one of them regular for $r \to 0$ and the other singular for $r \to 0$. For the physical problem, we need to select the regular solution. This determines $\psi_l(r)$ up to an overall normalizing constant.
Now let us now look at the wave function for large \( r \). Suppose that \( V(r) = 0 \) for \( r > R \). (This condition is not essential, but it makes our analysis simple. All that we really need is that \( V(r) \to 0 \) faster than \( 1/r \) for \( r \to \infty \).) Then \( \psi_+(\vec{x}) \) for \( r > R \) satisfies the free Schrödinger equation. The solutions of this equation are the spherical Hankel functions,

\[
\begin{align*}
    h_1^{(1)}(kr) &= j_l(kr) + in_l(kr), \\
    h_1^{(2)}(kr) &= j_l(kr) - in_l(kr).
\end{align*}
\]  

(177)

These functions are quite simply related to exponential functions

\[
\begin{align*}
    h_1^{(1)}(z) &= -iz^l \left( -\frac{1}{z} \frac{d}{dz} \right)^l \frac{1}{z} e^{iz}, \\
    h_1^{(2)}(z) &= iz^l \left( -\frac{1}{z} \frac{d}{dz} \right)^l \frac{1}{z} e^{-iz}.
\end{align*}
\]  

(178)

Thus \( h_1^{(1)}(kr) \) contains a polynomial in \( 1/(kr) \) times an outgoing spherical wave \( \exp(ikr) \), while \( h_1^{(2)}(kr) \) contains a polynomial in \( 1/(kr) \) times an incoming spherical wave \( \exp(-ikr) \).

Thus for \( r > R \) we must have

\[
\psi_l(r) = c_+^l h_1^{(1)}(kr) + c_-^l h_1^{(2)}(kr). \]  

(179)

Here \( c_+^l \) and \( c_-^l \) are constants. The overall normalization is not fixed by the differential equation, so one could multiply both \( c_+^l \) and \( c_-^l \) by the same constant. However, \( c_+^l / c_-^l \) is fixed by the differential equation.

One might solve the radial Schrödinger equation numerically. A standard method for doing that is to rewrite the radial Schrödinger equation as a first order differential equation for two functions, \( \psi_l(r) \) and \( d\psi_l(r)/dr \). Then we would approximate the differential equation as a finite difference equation using a step size \( \Delta r \) and solve the difference equation recursively starting near \( r = 0 \). The result is that we would find \( \psi_l(r) \) and \( d\psi_l(r)/dr \) for \( r \) outside the range of the potential. Then we could match \( \psi_l(r) \) and \( d\psi_l(r)/dr \) to Eq. (179) and find the coefficients \( c_+^l \) and \( c_-^l \).

In the following section, we see what this means for the scattering amplitude.
18 Relation to the phase shift

To relate our solution (179) to the scattering phase shift, we begin with Eq. (116), which applies when \( r \) is large enough that not only is \( V(r) \) small enough to neglect, but also \( kr \gg 1 \). We have

\[
(2\pi)^{3/2} \psi_+(r\vec{n}) \sim e^{ikr\cos\theta} + \frac{1}{r} e^{ikr} f(k\vec{n}, k\hat{z}) .
\] (180)

For \( f(k\vec{n}, k\hat{z}) \), we can use the partial wave expansion (164),

\[
f(\vec{k}_F, \vec{k}_I) = \sum_l (2l + 1) P_l(\cos\theta) f_l(k_I) .
\] (181)

With Eq. (174), this becomes

\[
f(\vec{k}_F, \vec{k}_I) = \frac{1}{2ik} \sum_l (2l + 1) P_l(\cos\theta) \left[ e^{2i\delta_l(k)} - 1 \right] .
\] (182)

Thus

\[
(2\pi)^{3/2} \psi_+(\vec{x}) \sim e^{ikr\cos\theta}
\]

\[
+ \sum_l (2l + 1) P_l(\cos\theta) \frac{1}{2ikr} e^{ikr} \left[ e^{2i\delta_l(k)} - 1 \right] .
\] (183)

This applies for \( kr \gg 1 \). We can relate this form to the structure of \( \psi_+(\vec{x}) \) when \( r \) is greater than the range \( R \) of the potential, even if \( kr \) is not large compared to 1. To do that, we consider

\[
\phi(\vec{x}) = (2\pi)^{3/2} \psi_+(r\vec{n}) - e^{ikr\cos\theta} .
\] (184)

For \( r > R \), this function obeys the free Schrödinger equation, so if we expand it in partial waves, the coefficient of \( P_l(\cos\theta) \) obeys the free radial Schrödinger equation and is thus a linear combination of \( h_l^{(1)}(kr) \) and \( h_l^{(2)}(kr) \). For \( kr \gg 1 \), these become

\[
h_l^{(1)}(kr) \sim \frac{(-i)^l}{ikr} e^{ikr} \quad r \to \infty ,
\]

\[
h_l^{(2)}(kr) \sim -\frac{(+i)^l}{ikr} e^{-ikr} \quad r \to \infty .
\] (185)
Our factor \((1/2ikr)e^{ikr}\) in Eq. (183) is just the large \(kr\) behavior of \(h^{(1)}_l(kr)\) times \(i^l/2\):
\[
\frac{i^l}{2} h^{(1)}_l(kr) \sim \frac{1}{2ikr} e^{ikr} \quad r \to \infty ,
\]
(186)

Eq. (183) has no term \((1/2ikr)e^{-ikr}\) in the expansion of \(\phi(\vec{x})\), so there is no \(h^{(2)}_l(kr)\) term. Thus \(\psi_+(\vec{x})\) must have the form
\[
(2\pi)^{3/2}\psi_+(\vec{x}) \sim e^{ikr\cos \theta}
\]
\[
+ \sum_l (2l + 1) P_l(\cos \theta) \frac{i^l}{2} h^{(1)}_l(kr) \left[e^{2i\delta_l(k)} - 1\right]
\]
for \(r\) big enough that \(V(r) = 0\) (or \(V(r)\) is small enough to be neglected).

For \(\exp(ikr\cos \theta)\), we can use Eq. (160)
\[
e^{ikr\cos \theta} = \sum_l (2l + 1) P_l(\cos \theta) i^l j_l(kr)
\]
\[
= \sum_l (2l + 1) P_l(\cos \theta) \frac{i^l}{2} \left[h^{(1)}_l(kr) + h^{(2)}_l(kr)\right]
\]
(188)

This gives
\[
(2\pi)^{3/2}\psi_+(\vec{x}) \sim \sum_l (2l + 1) P_l(\cos \theta) \frac{i^l}{2} \left[h^{(1)}_l(kr) + h^{(2)}_l(kr)\right]
\]
\[
+ \sum_l (2l + 1) P_l(\cos \theta) \frac{i^l}{2} h^{(1)}_l(kr) \left[e^{2i\delta_l(k)} - 1\right] .
\]
(189)

Thus we obtain
\[
(2\pi)^{3/2}\psi_+(\vec{x}) \sim \sum_l (2l + 1) P_l(\cos \theta) \frac{i^l}{2} \left[e^{2i\delta_l(k)} h^{(1)}_l(kr) + h^{(2)}_l(kr)\right]
\]
(190)
or
\[
\psi_l(r) = e^{2i\delta_l(k)} h^{(1)}_l(kr) + h^{(2)}_l(kr) .
\]
(191)

If there were no potential, then we would have just the plane wave \(e^{ikr\cos \theta}\) and would replace \(e^{2i\delta_l(k)} \to 1\) in Eq. (191). Two terms then would represent the outgoing wave part and the incoming wave part of the plane wave. With
a potential, the incoming wave part is unchanged, but now the outgoing wave part gets a phase $e^{2i\delta_l(k)}$.

Comparing to the $r > R$ form of our solution of the radial Schrödinger equation, Eq. (179), we see that if we normalize the solution so that $c_l^- = 1$ then

$$c_l^+ = e^{2i\delta_l(k)}.$$  \hspace{1cm} (192)

**Exercise 18.1** Find the phase shifts $\delta_l(k)$ for a hard sphere potential

$$V(r) = \begin{cases} 
\infty & r < a \\
0 & r > a
\end{cases}.$$  \hspace{1cm} (193)

Evaluate your result for the case $l = 0$.  

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