

Some Notes on Scattering

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Chapter 1

Introduction

<< Much of what we know about the fundamental forces of Nature has been learned from scattering experiments, in which essentially a target is bombarded with a beam of particles. Well-known examples are electron-positron, electron-proton and proton-antiproton scattering. But many other beam and/or target particles have been and are presently used in a rich variety of different types of experiments. The most famous perhaps of all scattering experiments is the dispersion of alpha particles on gold atoms, performed by Rutherford and his collaborators in the beginning of the 20th century.

Usually we know the nature of the particles used as projectiles, their energy and momentum, and perhaps their polarization. These particles are scattered by the target and subsequently, at distances large compared to the size of the target, detected by devices that may give us the intensity as a function of the direction of scattering.

From the theoretical point of view the most significant aspect of scattering processes is that we are concerned with the continuous part of the energy spectrum. We are free to choose the energy of the incident particles. Consequently, our interest is focused on the prediction of intensities since they are the object of measurement, rather than inspecting a Schrödinger equation for its eigenvalues.

Intensities, being measures of the likelihood of finding a particle at certain places, are of course related to the eigenfunctions. But, the connection between eigenfunctions and measured intensities is recondite and indirect. Scattering data can be compared with theoretical predictions only if we elucidate carefully the various stages of a scattering process. Relating observed intensities to calculated wave functions or transition probabilities, is the first problem of scattering theory.

In an idealized scattering experiment a single fixed scattering center is bombarded by particles incident along the z -axis. It is assumed that the effect of the scattering center on the particles can be represented by some kind of interaction, which is appreciably different from zero only within a finite region of small dimension.

Let us imagine a collimated homogeneous beam of monoenergetic particles moving toward the scatterer from a great distance. The width of the beam could be determined by slits, which although quite narrow from an experimental point of view (millimeters or even micrometers), are nevertheless very wide compared with the spatial extension of the scattering region (Fermies to Ångströms). Experimentally, in the interest of securing good statistics, which is the maximum number of counts in a given period of operation, it is desirable to employ intense beams. Yet the beam density must be low enough so that it can safely be assumed that the incident particles do not interact with one another.

After scattering, the particles are detected at a great distance from the scatterer. The detector subtends a cone of solid angle $d\Omega$ at the origin, where the target is placed, and the particles scattered into this cone are counted. If I_0 is the number of incident particles per unit area and $I d\Omega$ the number of these scattered into the cone, then we define the *differential scattering cross section* as

$$\frac{d\sigma}{d\Omega} = \frac{I(\vartheta, \varphi)}{I_0} . \quad (1.1)$$

This is the quantity which the experimentalist delivers to the theoretician. The latter interprets the cross section in terms of probabilities calculated from a theory. >>

(From chapter 11 of "Quantum Mechanics" by Eugen Merzbacher [1])

In this notes, which are not intended to be complete neither rigorous, we first study the non-relativistic Schrödinger formalism in order to set up a formal framework. In the second part we come to relativistic scattering, where not only high velocities, but also particle creation plays an important role.

Chapter 2

Wave packets

In quantum mechanics one describes a particle by a wave packet. Conceptually a wave packet may be first studied in one dimension. The generalization to three dimensions is straightforward and will be dealt with in a separate section.

2.1 One dimensional wave packet

Let us begin by studying an example: We indicate the position parameter in one dimension by x and the time by t . Let us assume that at the instant $t = 0$ a wave packet is given by the following expression (*Fourier expansion*):

$$\psi(x, t = 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) e^{ikx} \quad . \quad (2.1)$$

So, once the Fourier transform φ is specified we have an explicit example. The interpretation of the wave packet ψ , shown in formula (2.1), is the usual, *i.e.* the probability \mathcal{P} to find the particle, described by ψ , at the instant $t = 0$ at the position x is given by the square of the modulus of $\psi(x, t = 0)$ according to:

$$\mathcal{P}(x, t = 0) = |\psi(x, t = 0)|^2 \quad . \quad (2.2)$$

The example we will study here for φ , defined in formula (2.1), is a function of k which peaks around a certain value $k = \bar{k}$ and which vanishes rapidly for large values of $|k|$. For the sake of calculational simplicity we choose a Fourier transform which vanishes everywhere at the k -axis except for a small interval where it has a constant value different from zero, as is shown in figure (2.1a). In formula, the example for $\varphi(k)$ depicted in figure (2.1a), is represented by

$$\varphi(k) = \frac{1}{\sqrt{2\Delta k}} \theta \left((k - \bar{k})^2 - (\Delta k)^2 \right) = \begin{cases} \frac{1}{\sqrt{2\Delta k}} & , |k - \bar{k}| \leq \Delta k \\ 0 & , |k - \bar{k}| > \Delta k \end{cases} \quad (2.3)$$

The wave packet ψ which according to equation (2.1) follows for the above choice of Fourier transform φ can readily be determined to be given by

$$\psi(x, t = 0) = \frac{1}{\sqrt{\pi\Delta k}} e^{i\bar{k}x} \frac{\sin(\Delta k x)}{x} \quad , \quad (2.4)$$

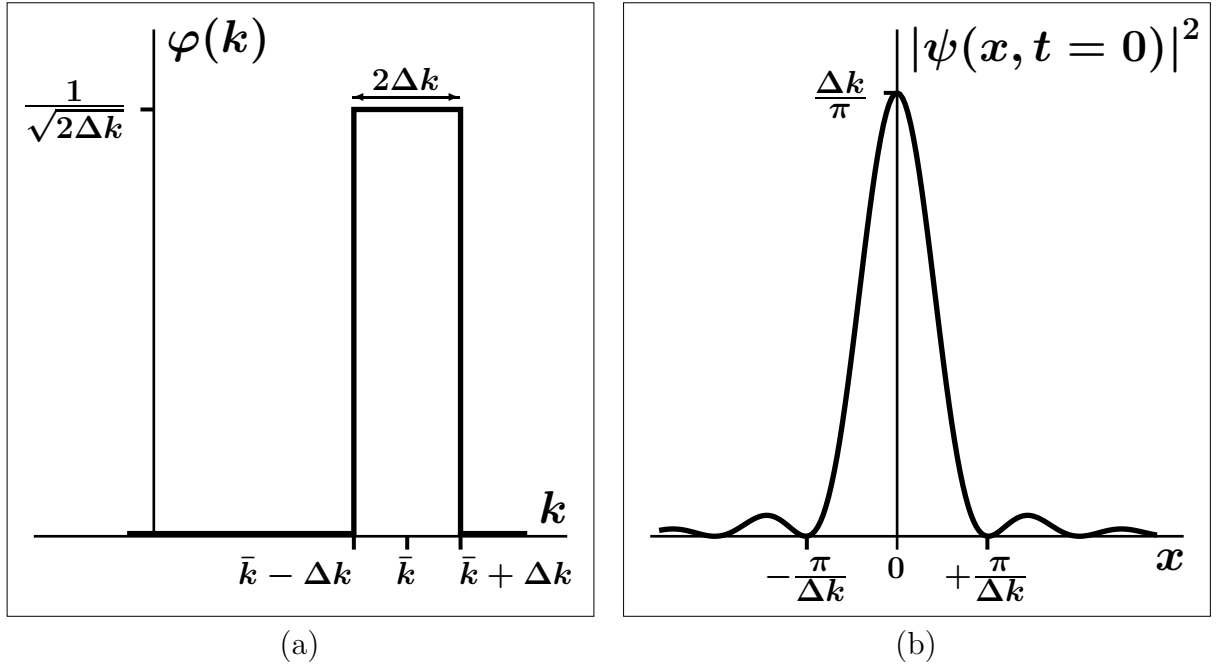


Figure 2.1: (a) The Fourier transform in one dimension of a wave packet which differs from zero only in a small region of width $2\Delta k$ around a central value $k = \bar{k}$. (b) The corresponding wave packet at the instant $t = 0$.

the probability distribution of which expression is depicted in figure (2.1b).

For completeness, let us go through the calculations which lead from formula (2.3), for our choice of Fourier transform, to expression (2.4): First notice that φ , given in formula (2.3), is normalized according to

$$\int_{-\infty}^{\infty} dk |\varphi(k)|^2 = \int_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} dk \frac{1}{2\Delta k} = 1 \quad . \quad (2.5)$$

This has as a consequence that the wave packet ψ , given in equation (2.1), is automatically normalized, which expresses the fact that the probability to find the particle somewhere along the x -axis equals 1 and can be seen from

$$\begin{aligned} \int_{-\infty}^{\infty} dx |\psi(x, t = 0)|^2 &= \int_{-\infty}^{\infty} dx \psi^*(x, t = 0)\psi(x, t = 0) = \\ &= \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi^*(k) e^{-ikx} \right\} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk' \varphi(k') e^{ik'x} \right\} \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \varphi^*(k) \varphi(k') \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{i(k' - k)x} \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \varphi^*(k) \varphi(k') \delta(k' - k) = \int_{-\infty}^{\infty} dk \varphi^*(k) \varphi(k) \\ &= \int_{-\infty}^{\infty} dk |\varphi(k)|^2 = 1 \quad . \end{aligned} \quad (2.6)$$

Performing the integral of formula (2.1) for the Fourier transform (2.3) is straightforward as we see:

$$\begin{aligned}
 \psi(x, t = 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) e^{ikx} = \frac{1}{2\sqrt{\pi\Delta k}} \int_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} dk e^{ikx} \\
 &= \frac{1}{2\sqrt{\pi\Delta k}} \frac{1}{ix} \left\{ e^{i(\bar{k} + \Delta k)x} - e^{i(\bar{k} - \Delta k)x} \right\} \\
 &= \frac{1}{\sqrt{\pi\Delta k}} e^{i\bar{k}x} \frac{\sin(\Delta k x)}{x} , \tag{2.7}
 \end{aligned}$$

which is right the function given in formula (2.4).

2.1.1 Momentum

In general a particle has velocity. So, we might wonder how velocity is represented by a wave packet. However, before studying the particle's dislocation in time we first determine its momentum. The time development of the wave packet we leave for a subsequent section.

The expectation value of momentum is in quantum mechanics defined by

$$\langle k \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \left\{ -i \frac{\partial}{\partial x} \right\} \psi(x) . \quad (2.8)$$

For the example (2.4) we obtain for the above expression the result

$$\langle k \rangle = \bar{k} . \quad (2.9)$$

The calculations can most easily be performed by following the same steps as in formula (2.6), *i.e.*

$$\begin{aligned} \langle k \rangle &= \int_{-\infty}^{\infty} dx \psi^*(x, t=0) \left\{ -i \frac{\partial}{\partial x} \right\} \psi(x, t=0) \\ &= \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi^*(k) e^{-ikx} \right\} \left\{ -i \frac{\partial}{\partial x} \right\} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk' \varphi(k') e^{ik'x} \right\} \\ &= \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi^*(k) e^{-ikx} \right\} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk' \varphi(k') k' e^{ik'x} \right\} \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \varphi^*(k) \varphi(k') k' \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{i(k' - k)x} \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \varphi^*(k) \varphi(k') k' \delta(k' - k) = \int_{-\infty}^{\infty} dk |\varphi(k)|^2 k \\ &= \int_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} dk \frac{k}{2\Delta k} = \bar{k} . \end{aligned} \quad (2.10)$$

We find thus that the most probable value to be measured for the particle's momentum, or the average value for a repeated number of measurements, equals \bar{k} which is indeed the central value of the k -distribution. As a consequence of this result one interprets the integration variable k in the Fourier expansion defined in formula (2.1) as the *momentum* of the Fourier component in the expansion. This has then moreover as a consequence that the time development of each Fourier component is different and thus in general that the wave packet tends to spread.

2.1.2 The Heisenberg uncertainty relation

By describing the motion of a particle by a wave packet, one introduces some uncertainty in the particle's position as well as some uncertainty in the particle's momentum. For instance, in the previous example as well the momentum distribution (2.3) as the position distribution (2.4) have some spreading. From figure (2.1a) we learn that the uncertainty in the momentum of the particle equals Δk , *i.e.*

$$k = \bar{k} \pm \Delta k \quad . \quad (2.11)$$

Moreover, from figure (2.1b) we may estimate that the width of the probability distribution equals about $\pi/\Delta k$, which amounts for the uncertainty in the particle's position to

$$\Delta x \approx \frac{\pi}{2\Delta k} \quad . \quad (2.12)$$

Consequently, for the product of the two uncertainties we obtain

$$\Delta k \Delta x \approx \frac{1}{2}\pi > \frac{1}{2} \quad , \quad (2.13)$$

for which we recognize the Heisenberg relation in units $\hbar = 1$.

2.1.3 The time development of a wave packet

The general expression for the time development of a wave packet is as follows:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) \exp \{i (kx - \omega(k)t)\} \quad , \quad (2.14)$$

where $\omega(k)$ is some function of momentum k .

In order to study the above expression (2.14), we assume that ω is linear in k , at least for values where the Fourier transform φ is maximal, *i.e.*

$$\omega(k) = \bar{\omega} + \bar{\omega}'(k - \bar{k}) \quad . \quad (2.15)$$

Such choice for ω leads for the wave packet (2.14) to the expression

$$\begin{aligned} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) \exp \left\{ i \left(kx - [\bar{\omega} + \bar{\omega}'(k - \bar{k})] t \right) \right\} \\ &= \frac{1}{\sqrt{2\pi}} \exp \left\{ i \left(-\bar{\omega}t + \bar{\omega}'\bar{k}t \right) \right\} \int_{-\infty}^{\infty} dk \varphi(k) \exp \{ ik (x - \bar{\omega}'t) \} \\ &= \exp \left\{ it \left(-\bar{\omega} + \bar{\omega}'\bar{k} \right) \right\} \psi(x - \bar{\omega}'t, 0) \quad , \end{aligned} \quad (2.16)$$

which implies that apart from a phase factor and a translation along the x -axis, the wave packet at the instant t has the same form as the wave packet at the instant $t = 0$. For the probability distribution one finds consequently

$$|\psi(x, t)|^2 = |\psi(x - \bar{\omega}'t, 0)|^2 \quad . \quad (2.17)$$

From the latter formula we read that the central peak in the probability distribution, which according to figure (2.1b) at $t = 0$ is found at the origin of the x -axis, is located at the position $x = \bar{\omega}'t$ at the instant of time t . Consequently, for ω linear in k as in formula (2.15), the wave packet moves with a constant velocity $\bar{\omega}'$ and hence represents a freely moving particle. The general idea is depicted in figure (2.2).

Notice, that for ω linear in k as in formula (2.15), the wave packet does not spread as time develops. A feature which at first sight also seems quite reasonable for a point particle in the absence of external forces. However, as we will see later on in subsection (2.1.5), in general ω is not linear in k as in formula (2.15). Hence, also quadratic and higher order terms must be considered which in general leads to spreading.

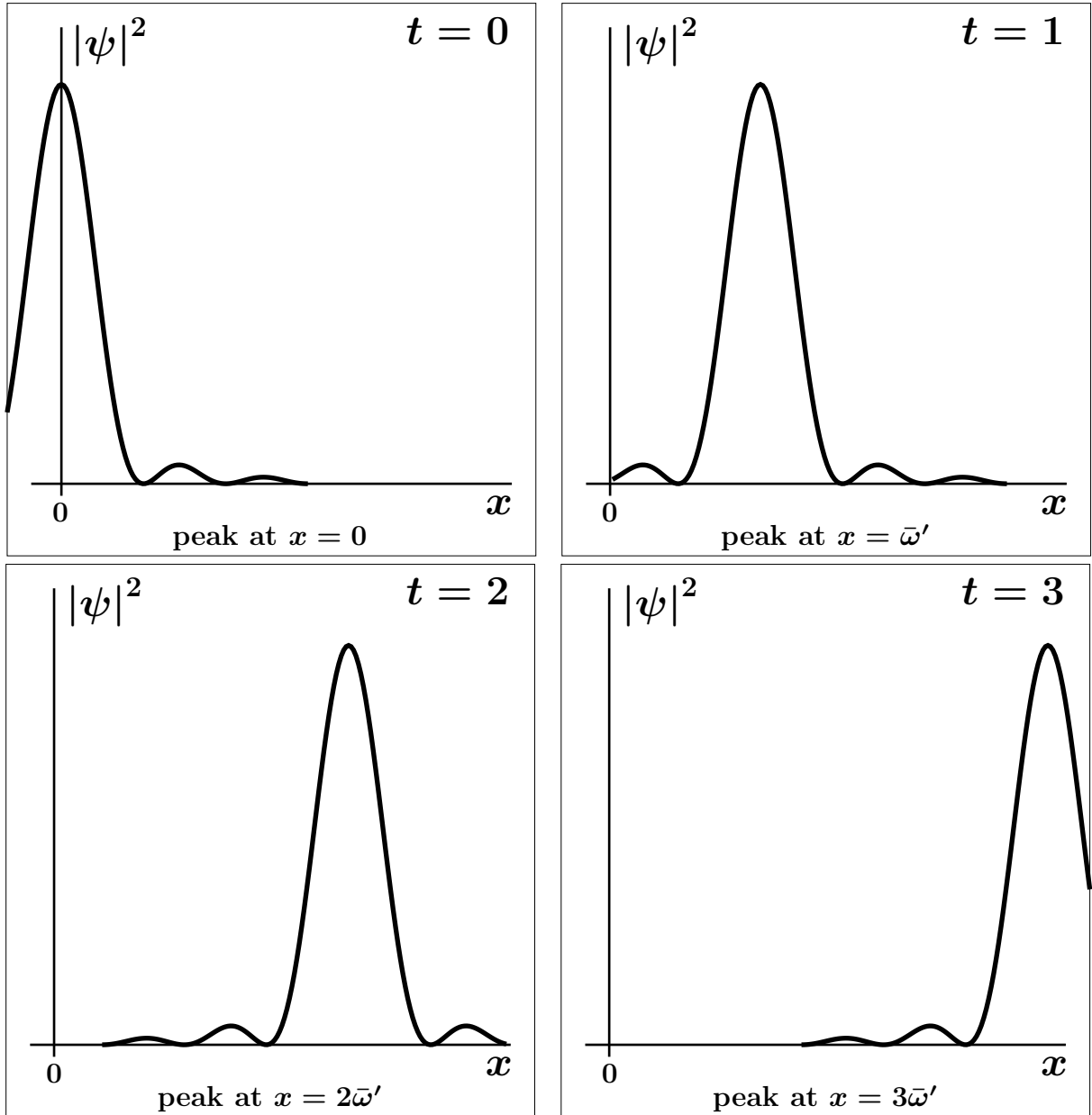


Figure 2.2: The probability distribution (2.17) in space (x) of wave packet (2.16) for the momentum distribution (2.3) at four different instances, $t = 0, 1, 2$ and 3 . The position of the maximum probability, which represents the most probable place where the particle can be found, moves at constant velocity $\bar{\omega}'$.

2.1.4 Energy

The expectation value of energy is in quantum mechanics related to the wave function's time development, and hence defined by

$$\langle E \rangle = \int_{-\infty}^{\infty} dx \psi^*(x, t) \left\{ i \frac{\partial}{\partial t} \right\} \psi(x, t) . \quad (2.18)$$

For the example (2.3) and moreover under the assumption that ω is linear in k as in formula (2.15), we obtain for the above expression the result

$$\langle E \rangle = \bar{\omega} . \quad (2.19)$$

The calculations can most easily be performed by following the same steps as in formula (2.8), *i.e.*

$$\begin{aligned} \langle E \rangle &= \int_{-\infty}^{\infty} dx \psi^*(x, t) \left\{ -i \frac{\partial}{\partial t} \right\} \psi(x, t) \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \varphi^*(k) \varphi(k') \omega(k') e^{i(\omega(k) - \omega(k'))t} \delta(k' - k) \\ &= \int_{-\infty}^{\infty} dk |\varphi(k)|^2 \omega(k) = \int_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} dk \frac{\bar{\omega} + \bar{\omega}'(k - \bar{k})}{2\Delta k} = \bar{\omega} . \end{aligned} \quad (2.20)$$

We find thus that the most probable value to be measured for the particle's energy, or the average value for a repeated number of measurements, equals $\bar{\omega}$, which is the central value for the momentum distribution (2.3), since from expression (2.15) one has

$$\omega(k = \bar{k}) = \bar{\omega} .$$

2.1.5 Momentum, velocity and energy

In the previous subsections we obtained for the wave packet representation (2.14) of a point particle, in the approximation that ω is linear in k as in formula (2.15), the following three results: The expectation values for the particle's momentum and energy are given in formulas (2.8) and (2.18) by respectively \bar{k} and $\bar{\omega} = \omega(\bar{k})$; whereas the particle's velocity is given by $\bar{\omega}'$. The latter quantity can more generally be written in the form (Taylor expansion coefficient):

$$\bar{\omega}' = \left(\frac{d\omega(k)}{dk} \right)_{k = \bar{k}} . \quad (2.21)$$

Now, in nonrelativistic mechanics we have the following relations between velocity v , momentum p , kinetic energy K and the particle's rest mass:

$$p = mv \quad \text{and} \quad K = \frac{p^2}{2m} . \quad (2.22)$$

In comparison, we would expect for the wave packet something similar. But, then we are dealing with distributions. Suppose, however, that the uncertainty in momentum is very small. In that case the variable k is for all Fourier components almost equal to its average or expectation value \bar{k} . The first of the two relations (2.22) would then translate into

$$\bar{\omega}' = \frac{\bar{k}}{m} , \quad (2.23)$$

whereas for the second relation one would expect

$$E \approx E(\bar{k}) = \frac{\bar{k}^2}{2m} . \quad (2.24)$$

This suggests that we may identify the time development function $\omega(k)$ defined in formula (2.14), with the energy variable $E(k)$ for each Fourier component. Formula (2.24) suggests then the choice

$$E(k) = \frac{k^2}{2m} . \quad (2.25)$$

A Taylor series expansion around the central value $k = \bar{k}$ of the latter expression for the k -dependence of the energy variable $E(k)$, gives us

$$\begin{aligned} E(k) = \omega(k) &= E(\bar{k}) + \left(\frac{dE}{dk} \right)_{k = \bar{k}} (k - \bar{k}) + \frac{1}{2} \left(\frac{d^2E}{dk^2} \right)_{k = \bar{k}} (k - \bar{k})^2 + \dots \\ &= \frac{\bar{k}^2}{2m} + \frac{\bar{k}}{m} (k - \bar{k}) + \frac{1}{2m} (k - \bar{k})^2 \end{aligned} \quad (2.26)$$

The above expansion is complete, since the higher order derivatives vanish. We may moreover observe that in case $\Delta k \ll \bar{k}$ one has that the third term in (2.26) is indeed much smaller than the second term. Hence, the assumption (2.15) is correct for such cases.

By comparing formula (2.15) to formula (2.26) we find from the first term indeed relation (2.24) and from the second term relation (2.23). Consequently, we may conclude that for the kinematics of a classical point particle the choice (2.25) is perfect.

2.1.6 Wave equation

Once the k -dependence of the energy variable $\omega(k) = E(k)$ has been settled, the wave equation follows immediately. When, for instance, we determine the first derivative in t for the wave packet (2.14), we find

$$i \frac{\partial}{\partial t} \psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) E(k) e^{i(kx - E(k)t)} . \quad (2.27)$$

Similarly, when we determine its second derivative in x , we obtain

$$\frac{\partial^2}{\partial x^2} \psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) (-k^2) e^{i(kx - E(k)t)} . \quad (2.28)$$

Consequently, from the k -dependence (2.25) for $E(k)$, we find for the wave packet (2.14) the wave equation

$$\begin{aligned} i \frac{\partial}{\partial t} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) E(k) e^{i(kx - E(k)t)} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) \frac{k^2}{2m} e^{i(kx - E(k)t)} \\ &= -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) , \end{aligned} \quad (2.29)$$

for which we recognize the Schrödinger equation in units $\hbar = 1$ for a system without interactions.

Notice, at this stage, that such wave equation just depends on our choice for the k -dependence for $E(k)$, in this case given by (2.25). Might we, for example, have preferred a k -dependence for $E(k)$ of the form

$$E(k) = \sqrt{k^2 + m^2} , \quad (2.30)$$

then we would have obtained for the wave equation of (2.14) the result

$$\begin{aligned} \frac{\partial^2}{\partial t^2} \psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) (-E^2(k)) e^{i(kx - E(k)t)} \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \varphi(k) (-k^2 - m^2) e^{i(kx - E(k)t)} \\ &= \left(\frac{\partial^2}{\partial x^2} - m^2 \right) \psi(x, t) , \end{aligned} \quad (2.31)$$

for which we recognize the Klein-Gordon equation in units $\hbar = 1$ for a system without interactions.

Consequently, the wave packet description in itself does not say anything about the dynamics of the system. It is just a consistent way of describing quantum mechanically the motion of a particle.

2.1.7 Plane wave

In the limit of vanishing Δk , one obtains a particle with a very well defined momentum, *i.e.* \bar{k} , but with a constant and thus vanishing probability distribution along the x -axis as can be seen, for instance by using formula (2.4), *i.e.*

$$\frac{1}{\sqrt{\pi\Delta k}} e^{i\bar{k}x} \frac{\sin(\Delta k x)}{x} \xrightarrow{\Delta k \rightarrow 0} \sqrt{\frac{\Delta k}{\pi}} e^{i\bar{k}x} . \quad (2.32)$$

The image of a particle being everywhere with the same probability and with a well-defined momentum, applies well to a beam of particles. One speaks then of a *plane wave* which has the form:

$$\psi(x) = \frac{e^{i\bar{k}x}}{\sqrt{2\pi}} . \quad (2.33)$$

The fact that a plane wave is not normalizable, can then be interpreted as describing the infinite number of particles in the beam.

2.2 Three dimensional wave packet

The generalization of the one dimensional wave packet (2.14) to three dimensions is straightforward. We define the position coordinates

$$x_1 , x_2 \text{ and } x_3 , \quad (2.34)$$

and similarly the three components of momentum

$$k_1 , k_2 \text{ and } k_3 . \quad (2.35)$$

and generalize wave packet (2.14) to a wave packet which describes a particle which moves in three dimensions by

$$\psi(\vec{x}, t) = \left(\frac{1}{2\pi}\right)^{3/2} \int d^3k \varphi(\vec{k}) \exp \left\{ i \left[\vec{k} \cdot (\vec{x} - \vec{x}_0) - E(\vec{k}) t \right] \right\} , \quad (2.36)$$

where \vec{x}_0 represents the "position" of the particle at $t = 0$.

2.2.1 Example

Let us study here the generalization to three dimensions of a Fourier transform φ which only differs appreciably from zero in a small area of momentum space surrounding a central value \vec{k} , *i.e.* a wave packet which represents a particle with "momentum" \vec{k} . In practice we will study the generalization of example (2.3), given by

$$\begin{aligned} \varphi(k) &= \prod_{i=1}^3 \frac{1}{\sqrt{2\Delta k_i}} \theta \left((k_i - \bar{k}_i)^2 - (\Delta k_i)^2 \right) \\ &= \begin{cases} \frac{1}{2\sqrt{2\Delta k_1 \Delta k_2 \Delta k_3}} & , |k_i - \bar{k}_i| \leq \Delta k_i \quad i = 1, \text{ and } i = 2, \text{ and } i = 3 \\ 0 & , |k_i - \bar{k}_i| > \Delta k_i \quad i = 1, \text{ or } i = 2, \text{ or } i = 3 \end{cases} \end{aligned} \quad (2.37)$$

It represents a function $\varphi(\vec{k})$ which vanishes everywhere in momentum space, except for the interior of a box with sides of length $2\Delta k_1$, $2\Delta k_2$ and $2\Delta k_3$ centered at \vec{k} .

The wave packet ψ , which according to equation (2.36) follows at the instant $t = 0$ for the above choice (2.37) of Fourier transform φ , can, by performing three times the same integration as shown in formula (2.7), readily be determined to be given by

$$\psi(\vec{x}, t = 0) = e^{i\vec{k} \cdot (\vec{x} - \vec{x}_0)} \prod_{i=1}^3 \frac{1}{\sqrt{\pi\Delta k_i}} \frac{\sin \left(\Delta k_i \left[\frac{x_i - (\vec{x}_0)_i}{\Delta k_i} \right] \right)}{x_i - (\vec{x}_0)_i} , \quad (2.38)$$

the probability distribution of which expression has a large maximum centered around \vec{x}_0 as in the three dimensional generalization of figure (2.1b).

2.2.2 Velocity and wave equation

Let us suppose that for a classical particle in three dimensions serves the generalization of the k -dependence for the energy E in one dimension as given in formula (2.25), i.e.

$$E(\vec{k}) = \frac{\vec{k}^2}{2m} \quad (2.39)$$

A Taylor series expansion of this expression around the central value \vec{k} gives us

$$\begin{aligned} E(\vec{k}) &= E(\vec{k}) + \sum_{i=1}^3 \left(\frac{\partial E}{\partial k_i} \right)_{\vec{k} = \vec{k}} (k_i - \bar{k}_i) + \dots \\ &= \frac{\vec{k}^2}{2m} + \frac{\vec{k}}{m} \cdot (\vec{k} - \vec{k}) + \dots \end{aligned} \quad (2.40)$$

When we restrict ourselves to the first two terms of this expansion, which for small values of Δk_1 , Δk_2 and Δk_3 leads to a very good approximation, then we obtain, following a similar calculus as in formula (2.16), for the probability distribution in coordinate space at the instant t the result

$$|\psi(\vec{x}, t)|^2 = \left| \psi \left(\vec{x} - \frac{\vec{k}}{m}t, 0 \right) \right|^2 . \quad (2.41)$$

From the latter formula we read that the central peak in the probability distribution, which at $t = 0$ is found at the position \vec{x}_0 , is located at the position $\vec{x} = \vec{x}_0 + \frac{\vec{k}}{m}t$ at the instant of time t . Consequently, the wave packet moves with a constant velocity $\frac{\vec{k}}{m}$ and hence represents a freely moving particle in three dimensions.

The *wave equation* which follows for the k -dependence of the energy given in formula (2.39), can be determined by a procedure similar to the one discussed in section (2.1.6), and yields

$$i \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\nabla^2}{2m} \psi(\vec{r}, t) \quad \text{where} \quad \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} , \quad (2.42)$$

for which one recognizes the three dimensional Schrödinger equation for a system without interactions.

2.2.3 Gaussian wave packet

Let us consider a Gaussian momentum distribution given by

$$\varphi(\vec{k}) = \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\frac{1}{2}\alpha(\vec{k} - \vec{k}_0)^2} . \quad (2.43)$$

It is easy to show that the distribution (2.43) is well normalised.

$$\begin{aligned} \int d^3k |\varphi(\vec{k})|^2 &= \int d^3k \left| \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\frac{1}{2}\alpha(\vec{k} - \vec{k}_0)^2} \right|^2 = \\ &= \left(\frac{\alpha}{\pi}\right)^{3/2} 4\pi \int_0^\infty k^2 dk e^{-\alpha k^2} = \left(\frac{\alpha}{\pi}\right)^{3/2} 4\pi \alpha^{-3/2} \frac{1}{2} \Gamma\left(\frac{3}{2}\right) = 1 . \end{aligned}$$

We will determine the time evolution of the wave packet which corresponds to the distribution (2.43). But, first let us determine the following Gaussian integral,

$$\begin{aligned} \int d^3k e^{-\frac{1}{2}A\vec{k}^2 + \vec{B} \cdot \vec{k}} &= \\ &= \int_{-\infty}^\infty dk_x e^{-\frac{1}{2}Ak_x^2 + B_x k_x} \int_{-\infty}^\infty dk_y e^{-\frac{1}{2}Ak_y^2 + B_y k_y} \int_{-\infty}^\infty dk_z e^{-\frac{1}{2}Ak_z^2 + B_z k_z} \\ &= \sqrt{\frac{2\pi}{A}} e^{B_x^2/2A} \sqrt{\frac{2\pi}{A}} e^{B_y^2/2A} \sqrt{\frac{2\pi}{A}} e^{B_z^2/2A} = \left(\frac{2\pi}{A}\right)^{3/2} e^{\vec{B}^2/2A} . \end{aligned} \quad (2.44)$$

The wave packet, which corresponds to the distribution (2.43), is given by

$$\begin{aligned} \psi(\vec{r}, t) &= \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) e^{i(\vec{k} \cdot \vec{r} - E(\vec{k})t)} = \\ &= \int \frac{d^3k}{(2\pi)^{3/2}} \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\frac{1}{2}\alpha(\vec{k} - \vec{k}_0)^2} e^{i(\vec{k} \cdot \vec{r} - E(\vec{k})t)} \\ &= \int \frac{d^3k}{(2\pi)^{3/2}} \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\frac{1}{2}\alpha\vec{k}^2 + \alpha\vec{k} \cdot \vec{k}_0 - \frac{1}{2}\alpha\vec{k}_0^2 + i\vec{k} \cdot \vec{r} - iE(\vec{k})t} . \end{aligned} \quad (2.45)$$

For $E(\vec{k}) = \vec{k}^2/2m$ we obtain for (2.45) the expression

$$\begin{aligned} \int \frac{d^3k}{(2\pi)^{3/2}} \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\frac{1}{2}\alpha\vec{k}^2 + \alpha\vec{k} \cdot \vec{k}_0 - \frac{1}{2}\alpha\vec{k}_0^2 + i\vec{k} \cdot \vec{r} - iE(\vec{k})t} &= \\ &= e^{-\frac{1}{2}\alpha\vec{k}_0^2} \left(\frac{\alpha}{\pi}\right)^{3/4} \int \frac{d^3k}{(2\pi)^{3/2}} e^{-\frac{1}{2}\left(\alpha + \frac{it}{m}\right)\vec{k}^2 + (\alpha\vec{k}_0 + i\vec{r}) \cdot \vec{k}} , \end{aligned} \quad (2.46)$$

which, by virtue of relation (2.44), equals

$$\psi(\vec{r}, t) = e^{-\frac{1}{2}\alpha\vec{k}_0^2} \left(\frac{\alpha}{\pi}\right)^{3/4} \left(\frac{1}{\alpha + \frac{it}{m}}\right)^{3/2} e^{\left\{\alpha\vec{k}_0 + i\vec{r}\right\}^2 / 2\left(\alpha + \frac{it}{m}\right)} . \quad (2.47)$$

First we work out the exponents.

$$\begin{aligned}
& -\frac{1}{2}\alpha\vec{k}_0^2 + \frac{\{\alpha\vec{k}_0 + i\vec{r}\}^2}{2\left(\alpha + \frac{it}{m}\right)} = \\
& = \frac{\left(\alpha^2\vec{k}_0^2 + 2i\alpha\vec{k}_0 \cdot \vec{r} - \vec{r}^2\right)\left(\alpha - \frac{it}{m}\right) - \alpha\vec{k}_0^2\left(\alpha^2 + \frac{t^2}{m^2}\right)}{2\left(\alpha^2 + \frac{t^2}{m^2}\right)} \\
& = \frac{-\alpha\left(\vec{r} - \frac{\vec{k}_0 t}{m}\right)^2 + i\alpha^2\left(2\vec{k}_0 \cdot \vec{r} - \left\{\vec{k}_0^2 + \alpha^{-2}\vec{r}^2\right\}\frac{t}{m}\right)}{2\left(\alpha^2 + \frac{t^2}{m^2}\right)} . \tag{2.48}
\end{aligned}$$

On substitution of the result (2.48) into relation (2.47), we obtain for the time development of a Gaussian wave packet

$$\begin{aligned}
\psi(\vec{r}, t) & = \left(\frac{1}{\pi\alpha}\right)^{3/4} \left(\frac{1}{1 + \frac{it}{\alpha m}}\right)^{3/2} \exp\left[\frac{-\alpha\left(\vec{r} - \frac{\vec{k}_0 t}{m}\right)^2}{2\left(\alpha^2 + \frac{t^2}{m^2}\right)}\right] \times \\
& \times \exp\left[\frac{i\alpha^2\left(2\vec{k}_0 \cdot \vec{r} - \left\{\vec{k}_0^2 + \alpha^{-2}\vec{r}^2\right\}\frac{t}{m}\right)}{2\left(\alpha^2 + \frac{t^2}{m^2}\right)}\right] . \tag{2.49}
\end{aligned}$$

For its probability distribution we find

$$|\psi(\vec{r}, t)|^2 = \left(\frac{1}{\pi\alpha\left(1 + \left\{\frac{t}{\alpha m}\right\}^2\right)}\right)^{3/2} \exp\left[-\frac{\left(\vec{r} - \frac{\vec{k}_0 t}{m}\right)^2}{\alpha\left(1 + \left\{\frac{t}{\alpha m}\right\}^2\right)}\right] . \tag{2.50}$$

The exponent in formula (2.50) has its peak value for

$$\vec{r} = \frac{\vec{k}_0}{m}t = \vec{v}_0 t . \tag{2.51}$$

Consequently, the peak value of $|\psi(\vec{r}, t)|^2$ moves with a constant velocity \vec{v}_0 . We furthermore notice that the width of the peak, which is given by

$$\sqrt{\alpha\left(1 + \left\{\frac{t}{\alpha m}\right\}^2\right)} , \tag{2.52}$$

grows in time, with a rate which is inversely proportional to the mass of the particle.

Chapter 3

Scattering

Let us consider the case in which a single fixed scattering center is bombarded by particles incident along the z -axis. In non-relativistic Schrödinger theory it is moreover assumed that the effect of the scattering center on the particles can be represented by a potential function $V(\vec{r})$, which is appreciably different from zero only within a finite region of dimensions a . By limiting ourselves to scattering from a potential we specialize to the case of elastic scattering, which is scattering without energy loss or gain by the projectile. However, many of the concepts developed here will be found useful in the discussion of inelastic collision processes and more general reactions.

For simplicity we shall suppose that the particles in the beam are all well represented by very broad and very long wave packets and that, before they reach the neighborhood of the scatterer, these packets can be described approximately by plane waves

$$e^{i(kz - \omega t)} \quad \text{where} \quad \omega = \frac{k^2}{2m} \quad , \quad (3.1)$$

although strictly speaking the waves do not extend to infinity either in width or in length.

In this chapter we will follow the procedure of how to obtain the differential scattering cross section from a given potential V , as outlined in chapter 11 of "Quantum Mechanics" by Eugen Merzbacher [1].

3.1 Scattering of wave packets

In the previous sections we only discussed wave packets which represent freely moving particles. One might therefore be curious of how systems with interaction can be described within this formalism.

Actually, there are two possibilities, which in a sense are equivalent, varying the k -dependence of $E(k)$, or varying the wave equations. As is usual, here we will represent interaction by a "potential" in the wave equation. For example, the extension of wave equation (2.42) to a wave equation for a system with interaction, is then given by

$$i\frac{\partial}{\partial t}\psi(\vec{r}, t) = H\psi(\vec{r}, t) = \left(-\frac{\nabla^2}{2m} + V(\vec{r})\right)\psi(\vec{r}, t) \quad . \quad (3.2)$$

The potential approach has the advantage that one can construct the wave equation in close analogy with a similar classical system, for which one knows how to formulate

a potential function. But, as a consequence, one has then to solve the resulting wave equation.

Here, we are interested in the scattering of particles from a target. So, we have an incident beam with a well-defined momentum, described by a plane wave, and outgoing waves which describe the scattered particles. We assume that this situation is well described by a potential which has a short range, *i.e.*:

$$V(\vec{r}) = 0 \quad \text{for} \quad r = |\vec{r}| > a \quad , \quad (3.3)$$

where a describes the dimension of the scatterer.

Let us assume that at $t = 0$ an incident particle of the beam is found at a distance r_0 away from the target and moving along the z -axis towards the target, which finds itself at the origin of the coordinate system. We assume moreover that r_0 is large with respect to the dimension of the target. In formula this implies for the position \vec{r}_0 of the projectile particle and its momentum \vec{k}_0 at the instant $t = 0$ that

$$\vec{r}_0 = -r_0 \hat{z} \quad \text{with} \quad r_0 \gg a \quad \text{and} \quad \vec{k}_0 = k_0 \hat{z} \quad (3.4)$$

Since at the position \vec{r}_0 the particle does not feel the potential, because of the conditions (3.3) and (3.4), we may describe its motion by a freely moving wave packet of the form

$$\psi(\vec{r}, 0) = \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) e^{i\vec{k} \cdot (\vec{r} - \vec{r}_0)} \quad , \quad (3.5)$$

where φ is a smooth function of narrow width, $\Delta\vec{k}$, centered around a mean momentum \vec{k}_0 . We assume r_0 to be so large that ψ at $t = 0$ has negligible probability density at the origin.

In section (3.6) we will show that the plane wave functions in the expansion (3.5) for the wave packet at $t = 0$ can be replaced by particular eigenfunctions $\psi^{(+)}$ of the Hamiltonian H , defined in formula (3.2), such that it obtains the form

$$\psi(\vec{r}, 0) = \int d^3k \varphi(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} \psi^{(+)}(\vec{k}, \vec{r}) \quad . \quad (3.6)$$

The retarded wave functions $\psi^{(+)}$ satisfy the stationary wave equation for the Hamiltonian H which has been defined in formula (3.2), *i.e.*

$$H\psi^{(+)}(\vec{k}, \vec{r}) = E\psi^{(+)}(\vec{k}, \vec{r}) \quad , \quad (3.7)$$

and, as we will see in section (3.5), have the following asymptotic behavior

$$\psi^{(+)}(\vec{k}, \vec{r}) \longrightarrow \frac{1}{(2\pi)^{3/2}} \left(e^{i\vec{k} \cdot \vec{r}} + f(\vec{k}, \hat{r}) \frac{e^{ikr}}{r} \right) \quad \text{for } r \text{ large} \quad , \quad (3.8)$$

which differs from a plane wave at large r only by an outgoing spherical wave. The function f is defined in formula (3.39).

Once it has been proven that the retarded wave functions $\psi^{(+)}$ exist and are eigenfunctions of the Hamiltonian H , defined in (3.2), then one has automatically solutions for the wave equation (3.2) by putting

$$\psi(\vec{r}, t) = \int d^3k \varphi(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}_0 - iEt) \psi^{(+)}(\vec{k}, \vec{r}) \quad \text{where } E = \frac{k^2}{2m} \quad . \quad (3.9)$$

Since the Hamiltonian (3.2) operates in coordinate space it can easily be verified that the above expression (3.9) is a solution of the wave equation (3.2), as

$$\begin{aligned} i \frac{\partial}{\partial t} \psi(\vec{r}, t) &= \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}_0 - iEt) E \psi^{(+)}(\vec{k}, \vec{r}) \\ &= \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}_0 - iEt) H \psi^{(+)}(\vec{k}, \vec{r}) \\ &= H \psi(\vec{r}, t) \quad . \end{aligned} \quad (3.10)$$

3.2 Differential scattering cross section

At $t = 0$ the contribution of the outgoing spherical wave is negligible. This fact will be studied in more detail in section (3.6). In formula (3.4) we defined the kinematic initial conditions for a projectile particle. In particular, we supposed that the particle is at a distance r_0 far away from the target at $t = 0$. Assuming that also the scattering detectors are at a macroscopic distance, of the order of r_0 , from the scatterer, we may conclude that the broad pulse will be traveling through the position of the detectors after a time

$$T = 2\frac{r_0}{v_0} = \frac{2mr_0}{k_0} \quad , \quad \text{where as in eq'n (2.22) } k_0 = mv_0 \quad . \quad (3.11)$$

When we examine the pulse at the position of the detectors, then $\psi^{(+)}$ can be represented by its asymptotic expansion (3.8). But, since the phases have changed with time, the outgoing spherical wave may no longer be neglected. However, we can make an approximation based on the identity

$$\begin{aligned} E(\vec{k}) &= \frac{k^2}{2m} = \frac{1}{2m} [\vec{k}_0 + (\vec{k} - \vec{k}_0)]^2 = \frac{1}{2m} \left\{ \vec{k}_0^2 + 2\vec{k}_0 \cdot (\vec{k} - \vec{k}_0) + (\vec{k} - \vec{k}_0)^2 \right\} \\ &= \vec{k} \cdot \frac{\vec{k}_0}{m} - \frac{\vec{k}_0^2}{2m} + \frac{(\vec{k} - \vec{k}_0)^2}{2m} = \vec{k} \cdot \vec{v}_0 - E_0 + \frac{(\vec{k} - \vec{k}_0)^2}{2m} \quad , \end{aligned} \quad (3.12)$$

where $E_0 = \vec{k}_0^2/2m$.

In order to be able to neglect the last term in expression (3.12), when E is substituted into (3.9), we require that the arrival time (3.11) at the scatterer, T , although large, should still satisfy the inequality

$$\frac{(\vec{k} - \vec{k}_0)^2}{2m} T \ll 1 \quad . \quad (3.13)$$

Now, since the relevant part of the \vec{k} -integration in (3.9) comes from an interval of width Δk around a mean value \vec{k}_0 (see formula (3.5)), we may, also substituting (3.11) for T , replace condition (3.13) by

$$\frac{(\Delta k)^2 r_0}{k_0} \ll 1 \quad . \quad (3.14)$$

This condition implies that the wave packet does not spread appreciable when it is displaced by the macroscopic distance r_0 .

Substituting the first two terms of (3.12) for E and the asymptotic expansion (3.8) for $\psi^{(+)}$ into the expression (3.9), we obtain the approximation

$$\psi(\vec{r}, t) \approx \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp[-i\vec{k} \cdot (\vec{r}_0 + \vec{v}_0 t) + iE_0 t] \left(e^{i\vec{k} \cdot \vec{r}} + f(\vec{k}, \hat{r}) \frac{e^{ikr}}{r} \right) \quad . \quad (3.15)$$

Assuming, moreover, that f , unlike φ , is a slowly varying function of \vec{k} , for (3.15) we can write

$$\begin{aligned} \psi(\vec{r}, t) \approx & e^{iE_0 t} \int \frac{d^3 k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp\left[i\vec{k} \cdot (\vec{r} - \vec{r}_0 - \vec{v}_0 t)\right] + \\ & + e^{iE_0 t} \frac{f(\vec{k}_0, \hat{r})}{r} \int \frac{d^3 k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp\left\{i\left[kr - \vec{k} \cdot (\vec{r}_0 + \vec{v}_0 t)\right]\right\} \end{aligned} \quad (3.16)$$

Since φ is appreciably different from zero only in an area of momentum space where $\hat{k} \approx \hat{k}_0$, we can substitute at the domain of integration for (3.16) effectively

$$kr \approx \vec{k} \cdot \hat{k}_0 r \quad ,$$

and consequently, obtain the further approximation

$$\begin{aligned} \psi(\vec{r}, t) \approx & e^{iE_0 t} \int \frac{d^3 k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp\left\{i\vec{k} \cdot [(\vec{r} - \vec{r}_0) - \vec{v}_0 t]\right\} + \\ & + e^{iE_0 t} \frac{f(\vec{k}_0, \hat{r})}{r} \int \frac{d^3 k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp\left\{i\vec{k} \cdot [(r\hat{k}_0 - \vec{r}_0) - \vec{v}_0 t]\right\} \end{aligned} \quad (3.17)$$

By comparing the above expression (3.17) to formula (3.5), we end up for (3.9) at the position of the detectors with the approximation

$$\psi(\vec{r}, t) \approx \psi(\vec{r} - \vec{v}_0 t, 0) e^{iE_0 t} + \frac{f(\vec{k}_0, \hat{r})}{r} \psi(r\hat{k}_0 - \vec{v}_0 t, 0) e^{iE_0 t} \quad . \quad (3.18)$$

Except for the phase factor $\exp(iE_0 t)$, the first term on the righthand side of (3.18) represents the initial wave packet displaced without change of shape, as if no scattering had occurred. This situation describes those projectile particles in the beam which had no interaction with the target constituents, and which consequently have no interest to the scattering experiment.

The second term on the righthand side of (3.18) is a scattered spherical wave packet, which describes the projectile particles which after interaction with the target move in all possible radial directions. As a function of time t the scattered spherical wave packet has the same form as the initial wave packet at time $t = 0$. This is indicated by the time-dependent function ψ . The amplitude, however, is reduced by a factor r^{-1} , which implies a reduction with a factor r^{-2} of the corresponding probability distribution as it should be for a spherically expanding density. The amplitude, moreover, is modulated by the angular amplitude $f(\vec{k}_0, \hat{r})$ which depends exclusively on the direction of scattering, not on the distance of the detector. Sensibly, the latter is called the *scattering amplitude*.

A detector outside the direction of the beam intercepts thus a radially expanding replica of the initial wave packet, equal to the one seen by the scatterer at the origin, but reduced in amplitude by a factor $f(\vec{k}_0, \hat{r})/r$. Now, let us assume that the detector has an area given by

$$r^2 d\Omega$$

perpendicular to the radial direction, and moreover that the probability distribution of the particle under consideration flows through that area with an average velocity given by v_0 . Then, in an infinitesimally small interval of time between t and $t + dt$, all probability contained in a volume given by

$$r^2 d\Omega \times v_0 dt$$

flows through the detector. Consequently, the probability of observing the scattered projectile particle at the detector in the time interval between t and $t + dt$ follows from

$$v_0 \left| \frac{f(\vec{k}_0, \hat{r})}{r} \right|^2 \left| \psi(r\hat{k}_0 - \vec{v}_0 t, 0) \right|^2 r^2 d\Omega dt = v_0 \left| f(\vec{k}_0, \hat{r}) \right|^2 d\Omega \left| \psi([r - v_0 t] \hat{k}_0, 0) \right|^2 dt. \quad (3.19)$$

Hence, the total probability for detecting it at the detector is

$$v_0 \left| f(\vec{k}_0, \hat{r}) \right|^2 d\Omega \int_{-\infty}^{+\infty} dt \left| \psi([r - v_0 t] \hat{k}_0, 0) \right|^2 = \left| f(\vec{k}_0, \hat{r}) \right|^2 d\Omega \int_{-\infty}^{+\infty} d\xi \left| \psi(\xi \hat{k}_0, 0) \right|^2, \quad (3.20)$$

where the limits of integration may be taken to be $-\infty$ and $+\infty$ with impunity, since ψ describes a wave packet of finite length.

On the other hand, the probability that the incident particle will pass through a unit area, located perpendicular to the beam in front of the scatterer, is

$$\int_{-\infty}^{+\infty} d\xi \left| \psi(\xi \hat{k}_0, 0) \right|^2. \quad (3.21)$$

Also here is no harm in extending the integration $-\infty$ to $+\infty$, since at $t = 0$ the wave packet is entirely in front of the scatterer.

If the ensemble contains N particles, all represented by the same general type of wave packet, then, using expression (3.20), we find that the number $I d\Omega$ of particles scattered into the solid angle $d\Omega$ is given by

$$I d\Omega = \left| f(\vec{k}_0, \hat{r}) \right|^2 d\Omega \sum_{i=1}^N \int_{-\infty}^{+\infty} d\xi \left| \psi_i(\xi \hat{k}_0, 0) \right|^2, \quad (3.22)$$

whereas, using formula (3.21), one has that

$$I_0 = \sum_{i=1}^N \int_{-\infty}^{+\infty} d\xi \left| \psi_i(\xi \hat{k}_0, 0) \right|^2. \quad (3.23)$$

gives the number of incident particles per unit area. Hence, by definition (1.1) we arrive at the fundamental result

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_0, \hat{r}) \right|^2. \quad (3.24)$$

3.3 The retarded Green's functions

Before we study the solutions $\psi^{(+)}$ of (3.7), we first study Green's functions. The Green's function, $G_+(\vec{r}, \vec{r}')$, which suits us here is a solution of the following differential equation

$$\frac{1}{2m} (\nabla^2 + k^2) G(\vec{r}, \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}') \quad , \quad (3.25)$$

which is, amongst other solutions, solved by

$$G_+(\vec{r}, \vec{r}') = -\frac{m}{2\pi} \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \quad . \quad (3.26)$$

More correct would be to state that since equation (3.25) is a second order differential equation, it has two independent solutions. Any linear combination of those two solutions is a solution of equation (3.25). Below, we will see that the choice (3.26) gives us the correct boundary conditions.

In order to verify that the above Green's function (3.26) solves equation (3.25), we take the case $\vec{r}' = 0$ without loss of generality. First we determine the second derivative with respect to $x = x_1$ of expression (3.26) for $r \neq 0$, which gives

$$\frac{\partial^2}{\partial x^2} \frac{e^{ikr}}{r} = e^{ikr} \left\{ \frac{ik}{r^2} - \frac{1}{r^3} \right\} + x^2 e^{ikr} \left\{ -\frac{k^2}{r^3} - \frac{3ik}{r^4} + \frac{3}{r^5} \right\} \quad .$$

For $y = x_2$ and $z = x_3$ one obtains similar expressions. Their sum gives

$$\begin{aligned} \nabla^2 \frac{e^{ikr}}{r} &= 3e^{ikr} \left\{ \frac{ik}{r^2} - \frac{1}{r^3} \right\} + r^2 e^{ikr} \left\{ -\frac{k^2}{r^3} - \frac{3ik}{r^4} + \frac{3}{r^5} \right\} \\ &= -k^2 \frac{e^{ikr}}{r} \quad \text{for } r \neq 0 \quad . \end{aligned}$$

For $r = 0$ we integrate equation (3.25) over the interior of a sphere with radius R surrounding the origin of coordinate space. For the righthand side we obtain trivially

$$\int_{\text{sphere}} d^3r \left\{ \delta^{(3)}(\vec{r}) \right\} = 1 \quad . \quad (3.27)$$

The lefthand side of (3.25) takes some more work. Let us start with the second term, *i.e.*

$$\begin{aligned} \int_{\text{sphere}} d^3r k^2 \frac{e^{ikr}}{r} &= \int d\Omega \int_0^R r^2 dr k^2 \frac{e^{ikr}}{r} \\ &= 4\pi \left[e^{ikr} (1 - ikR) - 1 \right] \quad . \end{aligned} \quad (3.28)$$

The r -integration can here most easily be obtained by applying the following identity

$$\int r dr e^{ikr} = -i \frac{\partial}{\partial k} \int dr e^{ikr} \quad .$$

Next we integrate the first term of the lefthand side of (3.25) by using the theorem of divergence, leading to

$$\begin{aligned} \int_{\text{sphere}} d^3r \nabla^2 \frac{e^{ikr}}{r} &= \int_{\text{surface}} d\vec{S} \cdot \vec{\nabla} \frac{e^{ikr}}{r} \\ &= 4\pi e^{ikR} (ikR - 1) . \end{aligned} \quad (3.29)$$

In the last step of formula (3.29) we used

$$d\vec{S} = R^2 d\Omega \hat{r} \quad \text{and} \quad \vec{\nabla} \frac{e^{ikr}}{r} = \hat{r} \frac{d}{dr} \frac{e^{ikr}}{r} .$$

When we put together the results (3.28) and (3.29), then we obtain for the integration on the interior of a sphere with radius R of the lefthand side of formula (3.25) the result

$$\int_{\text{sphere}} d^3r (\nabla^2 + k^2) \left(-\frac{1}{4\pi} \frac{e^{ikr}}{r} \right) = 1 . \quad (3.30)$$

Comparing the results (3.27) and (3.30) with equation (3.25) shows perfect agreement.

We may thus conclude that function (3.26) is a solution of the differential equation (3.25). It is referred to in the literature as the *retarded* Green's function.

3.4 Lippmann Schwinger equation for the wave function

The time-independent Schrödinger equation, which is related to the wave equation (3.2), is given by

$$\left[-\nabla^2 + 2mV(\vec{r})\right] \psi(\vec{r}) = k^2 \psi(\vec{r}) \quad . \quad (3.31)$$

A formal solution to this equation is given by the following expression

$$\psi^{(+)}(\vec{k}, \vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} + \int d^3r' G_+(\vec{r}, \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad , \quad (3.32)$$

as, using formula (3.25), can most easily be seen by performing

$$\begin{aligned} \frac{1}{2m} (\nabla^2 + k^2) \psi^{(+)}(\vec{k}, \vec{r}) &= \frac{1}{2m} (\nabla^2 + k^2) \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} + \\ &\quad + \int d^3r' \frac{1}{2m} (\nabla^2 + k^2) G_+(\vec{r}, \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \\ &= 0 + \int d^3r' \delta^{(3)}(\vec{r} - \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \\ &= V(\vec{r}) \psi^{(+)}(\vec{k}, \vec{r}) \quad , \end{aligned}$$

which leads exactly to equation (3.31).

Equation (3.32) is in fact an integral equation which substitutes the differential equation (3.31) incorporating the correct boundary conditions (as we will see in section (3.6)). In the literature it is referred to as the *Lippmann Schwinger* equation.

In order to see that the Lippmann Schwinger equation solves in principle equation (3.31), we first simplify the expression (3.32) by defining

$$\phi(\vec{k}, \vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} \quad , \quad (3.33)$$

which leads for (3.32) to

$$\psi^{(+)}(\vec{k}, \vec{r}) = \phi(\vec{k}, \vec{r}) + \int d^3r' G_+(\vec{r}, \vec{r}') V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad . \quad (3.34)$$

In the latter expression we substitute $\psi^{(+)}$ in the righthand side, to find

$$\begin{aligned} \psi^{(+)}(\vec{k}, \vec{r}) &= \phi(\vec{k}, \vec{r}) + \int d^3r' G_+(\vec{r}, \vec{r}') V(\vec{r}') \times \\ &\quad \times \left[\phi(\vec{k}, \vec{r}') + \int d^3r'' G_+(\vec{r}', \vec{r}'') V(\vec{r}'') \psi^{(+)}(\vec{k}, \vec{r}'') \right] \quad . \end{aligned}$$

Continuing this procedure leads to

$$\begin{aligned}
\psi^{(+)}(\vec{k}, \vec{r}) &= \phi(\vec{k}, \vec{r}) + \int d^3r_1 G_+(\vec{r}, \vec{r}_1) V(\vec{r}_1) \phi(\vec{k}, \vec{r}_1) + \\
&+ \int d^3r_1 \int d^3r_2 G_+(\vec{r}, \vec{r}_1) V(\vec{r}_1) G_+(\vec{r}_1, \vec{r}_2) V(\vec{r}_2) \phi(\vec{k}, \vec{r}_2) + \\
&+ \int d^3r_1 \int d^3r_2 \int d^3r_3 G_+(\vec{r}, \vec{r}_1) V(\vec{r}_1) G_+(\vec{r}_1, \vec{r}_2) V(\vec{r}_2) G_+(\vec{r}_2, \vec{r}_3) V(\vec{r}_3) \phi(\vec{k}, \vec{r}_3) + \\
&+ \dots \quad . \tag{3.35}
\end{aligned}$$

For a weak potential V this series converges and leads to a unique solution for $\psi^{(+)}$.

3.5 Asymptotic behaviour

When we substitute the expression (3.26) for the retarded Green's function into the Lipmann Schwinger equation (3.32), then we obtain

$$\psi^{(+)}(\vec{k}, \vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} - \frac{m}{2\pi} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad . \quad (3.36)$$

According to formula (3.3) the potential V vanishes at large distances, hence the domain of the \vec{r}' integral is located just around the origin within a sphere of radius a , *i.e.*

$$r' < a \quad . \quad (3.37)$$

Consequently, at distances r large compared to the target size a , such that

$$\frac{ka^2}{r} \ll 1 \quad ,$$

which implies only very small variations in the phases due to the quadratic and higher terms of the exponent, we may to first order in r' approximate

$$\begin{aligned} |\vec{r}-\vec{r}'| &= \sqrt{(\vec{r}-\vec{r}')^2} = \sqrt{r^2 + r'^2 - 2\vec{r} \cdot \vec{r}'} = r \sqrt{1 - \frac{(2\vec{r}-\vec{r}') \cdot \vec{r}'}{r^2}} \\ &\approx r \sqrt{1 - 2\frac{\hat{r} \cdot \vec{r}'}{r}} \approx r \left\{ 1 - \frac{\hat{r} \cdot \vec{r}'}{r} \right\} \approx r - \hat{r} \cdot \vec{r}' \quad . \end{aligned} \quad (3.38)$$

If, further, \vec{r}' in the denominator of the integrand is neglected, which can be done since $|\vec{r}-\vec{r}'|$ is smooth for $r \gg a$, we obtain for large r

$$\psi^{(+)}(\vec{k}, \vec{r}) \approx \frac{1}{(2\pi)^{3/2}} \left(e^{i\vec{k} \cdot \vec{r}} + \frac{e^{ikr}}{r} f(\vec{k}, \hat{r}) \right) \quad (r \text{ large})$$

where

$$f(\vec{k}, \hat{r}) = -\sqrt{2\pi} m \int d^3r' e^{-ik\hat{r} \cdot \vec{r}'} V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad \text{and} \quad k = |\vec{k}| \quad . \quad (3.39)$$

3.6 Initial conditions

Finally, it is left to be studied why the expansion (3.6) is correct. Using the explicit expression for $\psi^{(+)}$, given in formula (3.36), we obtain for (3.6)

$$\begin{aligned}
\psi(\vec{r}, 0) &= \int d^3k \varphi(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} \times \\
&\times \left[\frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} - \frac{m}{2\pi} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \right] \\
&= \int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\vec{k} \cdot \vec{r}} + \\
&- \int \frac{d^3k}{4\pi} \varphi(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} \frac{m}{2\pi} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad . \quad (3.40)
\end{aligned}$$

At $t = 0$, as affirmed in relation with formula (3.6), the second term in the righthand side of (3.40) vanishes, since the first term at the righthand side already equals the expression for the wave packet at $t = 0$ as given in formula (3.5). Now, since $U = 0$ for $r' > a$, it is sufficient to show that

$$\int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}_0 + ik|\vec{r}-\vec{r}'|) \psi^{(+)}(\vec{k}, \vec{r}') = 0 \quad (3.41)$$

for $r' < a$. It may usually be assumed that in this integral the variation of $\psi^{(+)}$ with \vec{k} can be neglected. Moreover, φ is appreciably different from zero only for vectors \vec{k} near the direction of \vec{k}_0 . Hence, we may approximate

$$k|\vec{r}-\vec{r}'| \approx \hat{k}_0 \cdot \vec{k} |\vec{r}-\vec{r}'|$$

and consequently, by comparing the result to formula (3.5), we find that the relevant part of the lefthand side of relation (3.41) is nearly equal to

$$\int \frac{d^3k}{(2\pi)^{3/2}} \varphi(\vec{k}) \exp\{i\vec{k} \cdot (\hat{k}_0 |\vec{r}-\vec{r}'| - \vec{r}_0)\} = \psi(\hat{k}_0 |\vec{r}-\vec{r}'|, 0) \quad .$$

The righthand side of this expression vanishes, because $\hat{k}_0 |\vec{r}-\vec{r}'|$ points to a position behind the scatterer where at $t = 0$ the wave packet was assumed to vanish.

3.7 Spherical well

In this section we consider the example of S -wave ($\ell = 0$) scattering from a spherical well, given by the following second order differential equation (in units $\hbar = c = 1$ and with the choice $2\mu = 1$ for the reduced mass of the scattered particles)

$$\left(-\frac{d^2}{dr^2} + V(r) - E\right)u(r) = 0 \quad \text{where} \quad V(r) = \begin{cases} V_0 & , \quad 0 < r < a \\ 0 & , \quad r > a \end{cases} . \quad (3.42)$$

The general solutions of equation (3.42) are elementary:

For $0 < r < a$ one has linear combinations of

$$\cos(\kappa r) \quad \text{and} \quad \sin(\kappa r) , \quad \text{where} \quad \kappa^2 = E - V_0 . \quad (3.43)$$

Whereas, for $r > a$ one has linear combinations of

$$\cos(kr) \quad \text{and} \quad \sin(kr) , \quad \text{where} \quad k^2 = E . \quad (3.44)$$

Taking moreover into account the boundary condition, $u = 0$, at the origin ($r = 0$), then we obtain for a solution of equation (3.42), the form

$$u(r) = \begin{cases} A \sin(\kappa r) & , \quad 0 < r < a \\ B \sin(kr + \delta(E)) & , \quad r > a \end{cases} . \quad (3.45)$$

The normalization constants A and B in formula (3.45) are determined by the boundary conditions at $r = a$, *i.e.*

$$\left.\frac{du}{dr}\right|_{r \downarrow a} = \left.\frac{du}{dr}\right|_{r \uparrow a} \quad \text{and} \quad u(r \downarrow a) = u(r \uparrow a) , \quad (3.46)$$

which leads to equations

$$Bk \cos(ka + \delta(E)) = A\kappa \cos(\kappa a) \quad \text{and} \quad B \sin(ka + \delta(E)) = A \sin(\kappa a) . \quad (3.47)$$

By elimination of the normalization constants A and B in formula (3.47), we obtain

$$k \frac{\cotg(ka)\cotg(\delta(E)) - 1}{\cotg(\delta(E)) + \cotg(ka)} = \kappa \cotg(\kappa a) , \quad (3.48)$$

from which we can solve

$$\cotg(\delta(E)) = \frac{k + \kappa \cotg(\kappa a)\cotg(ka)}{k \cotg(ka) - \kappa \cotg(\kappa a)} . \quad (3.49)$$

Notice, that the righthand-side expression of formula (3.49) is real for real energy, E , even for cases where $\kappa^2 < 0$. In the latter cases one has

$$\kappa \cotg(\kappa a) = i\kappa \coth(i\kappa a) = i\kappa \frac{e^{i\kappa a} + e^{-i\kappa a}}{e^{i\kappa a} - e^{-i\kappa a}} ,$$

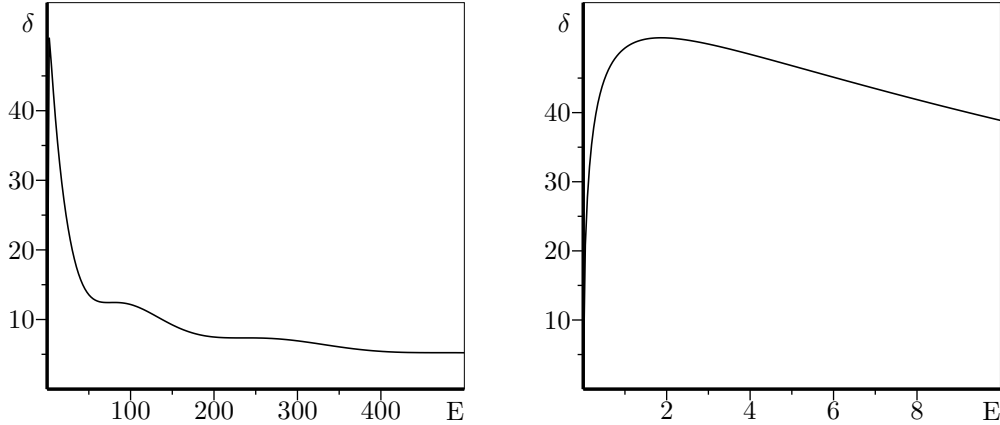


Figure 3.1: Phase shifts for a spherical well potential. For the depth, V_0 , and the width, a , of the well we have chosen here -8 and 0.5 respectively. The lefthand side picture shows the phase shifts for energies up to 500. Whereas, the righthand side picture exhibits the details for the phase shifts at low energies.

which is manifestly real for purely imaginary κ .

A typical example for the phase shifts of a spherical well is depicted in figure (3.1).

From relations (3.47), also using formula (3.49), one may moreover determine the ratio of the normalization constants A and B , *i.e.*

$$\frac{A}{B} = \frac{\sin(ka + \delta(E))}{\sin(\kappa a)} = \left(\sin^2(\kappa a) + \frac{\kappa^2}{k^2} \cos^2(\kappa a) \right)^{-\frac{1}{2}}. \quad (3.50)$$

The wave function (3.45) can then be obtained upto an overall normalization constant. An example has been depicted in figure (3.2). The lefthand side picture shows the wave function. Whereas the righthand side picture shows the continuation of each of the two different functions (3.45), one for $0 < r < a$ and one for $r > a$, into the r -interval where they do not coincide with the wave function. From the latter picture one observes more easily that at the boundary of the spherical well, $a = 0.5$ here, both the wave function and its derivative are continuous functions in r .

Notice that the function $B \sin(kr + \delta(E))$ which describes the part of the wave function for $r > a$ does not vanish at the origin, but instead results to $B \sin(\delta(E))$ for $r = 0$.

When $E < V_0$, then one may define the wave function in a slightly different way. Instead of expressions (3.45) we prefer for imaginary κ the following for the wave function

$$u(r) = \begin{cases} \frac{A'}{2} (e^{i\kappa r} - e^{-i\kappa r}) & , \quad 0 < r < a \\ B \sin(kr + \delta(E)) & , \quad r > a \end{cases}. \quad (3.51)$$

This has no effect for the phase shifts, whereas for the ratio of A' and B we obtain then

$$\frac{A'}{B} = \frac{\sin(ka + \delta(E))}{\frac{1}{2}(e^{i\kappa r} - e^{-i\kappa r})}. \quad (3.52)$$

An example has been depicted in figure (3.3).

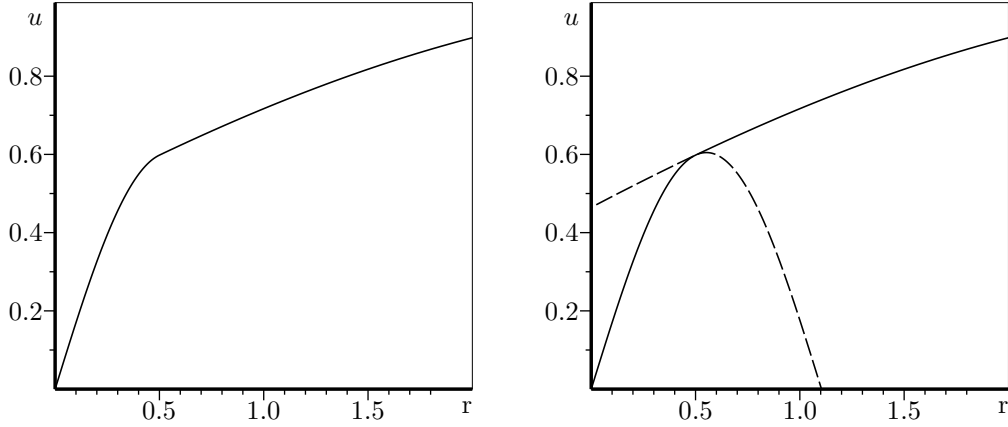


Figure 3.2: Wave function for the spherical well for $E = 0.1$. The intensity, V_0 , equals -8.0 , the width of the well, a , equals 0.5 . The wave function is not normalized. We took $A = 1$.

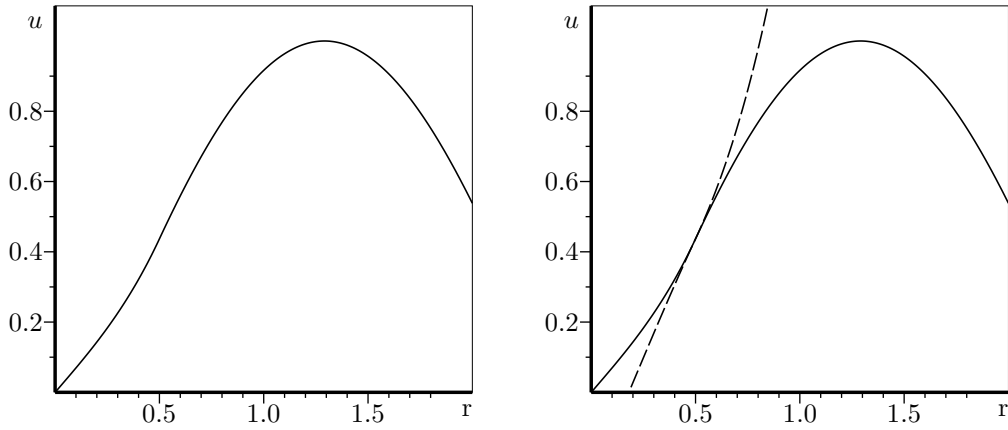


Figure 3.3: Wave function for the spherical well for $E = 2.0$. The intensity, V_0 , equals 8.0 , the width of the well, a , equals 0.5 . The wave function is not normalized. We took $A' = 1$.

3.7.1 The effective range expansion

We inspect the expression (3.49) for very low energies.

From formulae (3.43) and (3.44), we obtain

$$\kappa^2 \rightarrow \kappa_0^2 = -V_0 \quad \text{and} \quad k^2 \rightarrow 0 \quad , \quad (3.53)$$

when E tends to zero. Hence, for the cotangents of ka and κa , we obtain for very low energies the following approximations

$$\cotg(ka) \rightarrow \frac{1}{ka} \quad \text{and} \quad \cotg(\kappa a) \rightarrow \cotg(\kappa_0 a) \quad , \quad (3.54)$$

For expression (3.49) we find then

$$\cotg(\delta(E)) \rightarrow \frac{1}{ka} \frac{(ka)^2 + a\kappa_0 \cotg(\kappa_0 a)}{1 - a\kappa_0 \cotg(\kappa_0 a)} \quad , \quad (3.55)$$

or equivalently

$$k \cotg(\delta(E)) \rightarrow \frac{1}{a} \frac{a \kappa_0 \cotg(\kappa_0 a)}{1 - a \kappa_0 \cotg(\kappa_0 a)} + k^2 \frac{a}{1 - a \kappa_0 \cotg(\kappa_0 a)} , \quad (3.56)$$

The result (3.56) can be generalized to include a variety of interaction potentials and for different partial waves (ℓ):

$$k^{2\ell+1} \cotg(\delta(E)) = -\frac{1}{a_\ell} + \frac{1}{2} R_\ell k^2 + \dots , \quad (3.57)$$

an expansion entirely in k^2 . The parameters a_ℓ and R_ℓ are in the literature referred to by partial wave scattering length and effective range, respectively. Here, we will study some properties of a_0 , the S -wave scattering length for the spherical well potential.

By comparing formula (3.56) with formula (3.57), we find

$$a_0 = a \frac{a \kappa_0 \cotg(\kappa_0 a) - 1}{a \kappa_0 \cotg(\kappa_0 a)} . \quad (3.58)$$

On analyzing the following expression

$$F(x) = \frac{x \cotg(x) - 1}{x \cotg(x)} ,$$

we find that for reasonable values of a and V_0 the partial S -wave scattering length a_0 is positive for positive V_0 and negative for negative V_0 .

To lowest order in k^2 one obtains for the exterior part of the wave function (3.45), the expression

$$u(r > a) = B \sin(kr + \delta(E)) \rightarrow \frac{B \sin(\delta(E))}{a_0} (a_0 - r) , \quad (3.59)$$

which vanishes for $r = a_0$. A positive zero of the wave function, hence positive a_0 , can be observed for the case of a positive potential well in Figure (3.3), where the exterior wave function is continued into the interior ($r < a$). For a negative potential well we observe from Figure (3.2) that a zero of the exterior wave function takes place at negative values of r , hence negative a_0 .

3.7.2 One-delta-shell approximation

The system (3.42) may be approximated by a one-delta-shell potential, according to

$$\left(-\frac{d^2}{dr^2} + a V_0 \delta(r - b) - E \right) u(r) = 0 \quad \text{with} \quad 0 < b < a . \quad (3.60)$$

In the absence of any potential in both regions, $0 < r < b$ and $r > b$, the general solutions of differential equation (3.60) are there linear combinations of

$$\cos(kr) \quad \text{and} \quad \sin(kr) , \quad \text{where} \quad k^2 = E . \quad (3.61)$$

Hence, taking into account the boundary condition at the origin, we find the following solution for (3.60)

$$u(r) = \begin{cases} A \sin(kr) & , \quad 0 < r < b \\ B \sin(kr + \delta(E)) & , \quad r > b \end{cases} . \quad (3.62)$$

The boundary conditions at $r = b$ are different from those given in formula (3.46). By twice integrating the differential equation (3.60) in a small domain, $(b - \epsilon, b + \epsilon)$, around the delta-shell position $r = b$ and letting $\epsilon \rightarrow 0$, one finds

$$-\left. \frac{du}{dr} \right|_{r \downarrow b} + \left. \frac{du}{dr} \right|_{r \uparrow b} + aV_0 u(b) = 0 \quad \text{and} \quad u(r \downarrow b) = u(r \uparrow b) \quad , \quad (3.63)$$

which leads to equations

$$\begin{aligned} -Bk \cos(kb + \delta(E)) + Ak \cos(kb) + aV_0 A \sin(kb) &= 0 \\ \text{and} \quad B \sin(kb + \delta(E)) &= A \sin(kb) \quad . \end{aligned} \quad (3.64)$$

Elimination of the normalization constants, A and B , in formula (3.64), leads to an expression for the cotangent of the phase shifts, given by

$$\cotg(\delta(E)) = -\frac{\cos(kb)}{\sin(kb)} - \frac{k}{aV_0 \sin^2(kb)} \quad . \quad (3.65)$$

A typical example for the phase shifts of a spherical delta shell is depicted in figure (3.4).

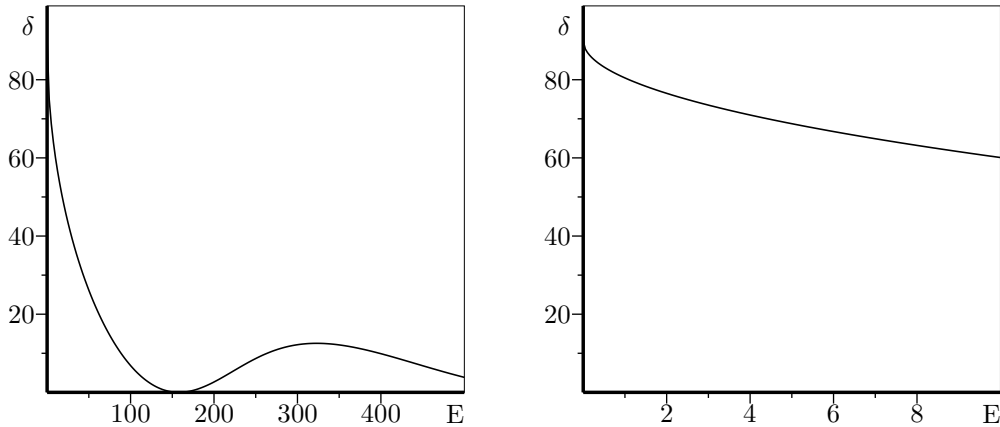


Figure 3.4: Phase shifts for the one-delta-shell potential as defined in formula (3.60). The intensity of the potential is given by aV_0 . We have chosen here the same values for a and V_0 , *i.e.* 0.5 and -8 respectively, as for the results depicted in figure (3.1). For the delta shell radius we have chosen here $b = \frac{1}{2}a$.

From relations (3.64) one may also here determine the ratio of the normalization constants A and B , *i.e.*

$$\frac{A}{B} = \frac{\sin(kb + \delta(E))}{\sin(kb)} \quad . \quad (3.66)$$

The wave function (3.62) can then be calculated upto an overall normalization constant. An example has been depicted in figure (3.5). The lefthand side picture shows the wave function for $E = 2.0$, the righthand side picture for $E = 10$.

Notice that now the wave function has a sharp discontinuity in its derivative with respect to r at the position of the delta shell. This corresponds to the first of the boundary conditions given in formula (3.63), which says that the difference in the derivatives from above $r \downarrow b$ and from below $r \uparrow b$ is proportional to the value of the wave function at $r = b$.

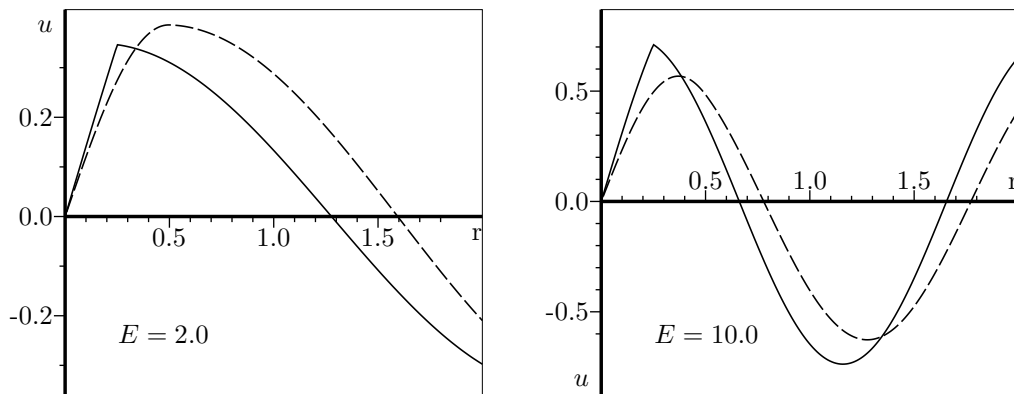


Figure 3.5: Wave functions for the one-delta-shell potential for $E = 2.0$ and $E = 10.0$. The intensity is given by $aV_0/$. The dashed line is the exact solution for the spherical well ($V_0 = -8.0$ and $a = 0.5$). The wave function is not normalized. We took $A = 1$.

3.7.3 A formal solution of the one-delta-shell potential

The solution (3.62) can formally be written in the form

$$\begin{pmatrix} u(r) \\ u'(r) \end{pmatrix} = \begin{pmatrix} \sin(kr) & -\frac{\cos(kr)}{k} \\ k \cos(kr) & \sin(kr) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}, \quad (3.67)$$

where $u'(r)$ stands for du/dr and where

$$\begin{cases} C = A \quad \text{and} \quad D = 0 & \text{for} \quad 0 < r < b \\ C = B \cos(\delta(E)) \quad \text{and} \quad D = -kB \sin(\delta(E)) & \text{for} \quad r > b \end{cases}. \quad (3.68)$$

Let us define the propagator, $\mathcal{G}(r_2, r_1)$, which connects the values of the wave function and of its derivatives at two different positions $r_1 < r_2$, as follows

$$\begin{pmatrix} u(r_2) \\ u'(r_2) \end{pmatrix} = \mathcal{G}(r_2, r_1) \begin{pmatrix} u(r_1) \\ u'(r_1) \end{pmatrix}. \quad (3.69)$$

This propagator has the following properties

$$\mathcal{G}(r_1, r_1) = \mathbf{1} \quad , \quad \mathcal{G}(r_3, r_1) = \mathcal{G}(r_3, r_2) \mathcal{G}(r_2, r_1) \quad \text{and} \quad \mathcal{G}^{-1}(r_2, r_1) = \mathcal{G}(r_1, r_2) \quad . \quad (3.70)$$

When there is no potential, *i.e.* $V(r) = 0$, in the interval from r_1 to r_2 , then it is easy to verify that a suitable choice for the propagator is given by

$$\mathcal{G}(r_2, r_1) = \begin{pmatrix} \sin(kr_2) & -\frac{\cos(kr_2)}{k} \\ k \cos(kr_2) & \sin(kr_2) \end{pmatrix} \begin{pmatrix} \sin(kr_1) & \frac{\cos(kr_1)}{k} \\ -k \cos(kr_1) & \sin(kr_1) \end{pmatrix} \quad . \quad (3.71)$$

Now, the boundary conditions (3.63) at $r = b$ can be written as

$$\begin{pmatrix} u(r \downarrow b) \\ u'(r \downarrow b) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ aV_0 & 1 \end{pmatrix} \begin{pmatrix} u(r \uparrow b) \\ u'(r \uparrow b) \end{pmatrix} \quad . \quad (3.72)$$

Hence, when we want to pass from one side of the delta shell to the other, *i.e.* from $r_1 < b$ to $r_2 > b$, then we may proceed as follows

$$\begin{aligned} \begin{pmatrix} u(r_2) \\ u'(r_2) \end{pmatrix} &= \mathcal{G}(r_2, r \downarrow b) \begin{pmatrix} u(r \downarrow b) \\ u'(r \downarrow b) \end{pmatrix} \\ &= \mathcal{G}(r_2, r \downarrow b) \begin{pmatrix} 1 & 0 \\ aV_0 & 1 \end{pmatrix} \begin{pmatrix} u(r \uparrow b) \\ u'(r \uparrow b) \end{pmatrix} \\ &= \mathcal{G}(r_2, r \downarrow b) \begin{pmatrix} 1 & 0 \\ aV_0 & 1 \end{pmatrix} \mathcal{G}(r \uparrow b, r_1) \begin{pmatrix} u(r_1) \\ u'(r_1) \end{pmatrix} \quad , \quad (3.73) \end{aligned}$$

which upon the use of formulas (3.71) and (3.72), takes the form

$$\begin{aligned} \begin{pmatrix} u(r_2) \\ u'(r_2) \end{pmatrix} &= \begin{pmatrix} \sin(kr_2) & -\frac{\cos(kr_2)}{k} \\ k \cos(kr_2) & \sin(kr_2) \end{pmatrix} \times \\ &\times \begin{pmatrix} 1 + \frac{aV_0}{k} \sin(kb) \cos(kb) & -\frac{aV_0}{k^2} \cos^2(kb) \\ aV_0 \sin^2(kb) & 1 - \frac{aV_0}{k} \sin(kb) \cos(kb) \end{pmatrix} \times \\ &\times \begin{pmatrix} \sin(kr_1) & \frac{\cos(kr_1)}{k} \\ -k \cos(kr_1) & \sin(kr_1) \end{pmatrix} \begin{pmatrix} u(r_1) \\ u'(r_1) \end{pmatrix} \quad , \quad (3.74) \end{aligned}$$

Formula (3.74) can easily be generalized for the case of more delta-shells. It just leads to repeated matrix multiplications as will be studied in section (3.7.4).

In the case of one delta shell at $r = b$ one has expressions (3.68) for the coefficients of the wave function in the two domains, $0 < r_1 < b$ and $r_2 > b$. This reduces formula (3.74) to

$$\begin{aligned}
& \begin{pmatrix} \sin(kr_2) & -\frac{\cos(kr_2)}{k} \\ k \cos(kr_2) & \sin(kr_2) \end{pmatrix} \begin{pmatrix} B \cos(\delta(E)) \\ -kB \sin(\delta(E)) \end{pmatrix} = \\
& = \begin{pmatrix} \sin(kr_2) & -\frac{\cos(kr_2)}{k} \\ k \cos(kr_2) & \sin(kr_2) \end{pmatrix} \times \\
& \quad \times \begin{pmatrix} 1 + \frac{aV_0}{k} \sin(kb) \cos(kb) & -\frac{aV_0}{k^2} \cos^2(kb) \\ aV_0 \sin^2(kb) & 1 - \frac{aV_0}{k} \sin(kb) \cos(kb) \end{pmatrix} \times \\
& \quad \times \begin{pmatrix} \sin(kr_1) & \frac{\cos(kr_1)}{k} \\ -k \cos(kr_1) & \sin(kr_1) \end{pmatrix} \begin{pmatrix} \sin(kr_1) & -\frac{\cos(kr_1)}{k} \\ k \cos(kr_1) & \sin(kr_1) \end{pmatrix} \begin{pmatrix} A \\ 0 \end{pmatrix}, \quad (3.75)
\end{aligned}$$

or equivalently, to

$$\begin{pmatrix} B \cos(\delta(E)) \\ -kB \sin(\delta(E)) \end{pmatrix} = \begin{pmatrix} 1 + \frac{aV_0}{k} \sin(kb) \cos(kb) & -\frac{aV_0}{k^2} \cos^2(kb) \\ aV_0 \sin^2(kb) & 1 - \frac{aV_0}{k} \sin(kb) \cos(kb) \end{pmatrix} \begin{pmatrix} A \\ 0 \end{pmatrix}. \quad (3.76)$$

For the phase shift we obtain then

$$\cotg(\delta(E)) = -\frac{\cos(kb)}{\sin(kb)} - \frac{k}{aV_0 \sin^2(kb)}, \quad (3.77)$$

which may be compared to formula (3.65).

3.7.4 Multi-delta-shell approximation

Let us consider an approximation of the potential (3.42) by more than one delta shell, *i.e.*

$$V(r) = V_0 \sum_{n=1}^N \Delta_n \delta(r - b_n), \quad (3.78)$$

where $0 < b_1 < b_2 < \dots < b_N < a$ and where $\Delta_1, \Delta_2, \dots, \Delta_N$ represent the measures which belong to the distribution $\{b_n \mid n = 1, \dots, N\}$. Let us, moreover, define the following matrices

$$X(b, \Delta) = \begin{pmatrix} 1 + \frac{\Delta V_0}{k} \sin(kb) \cos(kb) & -\frac{\Delta V_0}{k^2} \cos^2(kb) \\ \Delta V_0 \sin^2(kb) & 1 - \frac{\Delta V_0}{k} \sin(kb) \cos(kb) \end{pmatrix}, \quad (3.79)$$

and

$$\mathcal{X} = X(b_N, \Delta_N) \cdot \dots \cdot X(b_2, \Delta_2) \cdot X(b_1, \Delta_1). \quad (3.80)$$

Then, in passing over all delta-shell positions from $r_1 < b_1$ to $r_2 > b_N$, we obtain for the relations between the normalization constants, A and B , and the cosine and sine of the phase shift the expression

$$\begin{pmatrix} B \cos(\delta(E)) \\ -kB \sin(\delta(E)) \end{pmatrix} = \begin{pmatrix} \mathcal{X}_{11} & \mathcal{X}_{12} \\ \mathcal{X}_{21} & \mathcal{X}_{22} \end{pmatrix} \begin{pmatrix} A \\ 0 \end{pmatrix}, \quad (3.81)$$

which results for the cotangent of the phase shift in

$$\cotg(\delta(E)) = -k \frac{\mathcal{X}_{11}}{\mathcal{X}_{21}}. \quad (3.82)$$

Typical examples for the phase shifts of many-delta-shell approximations of the spherical well are depicted in figure (3.6), respectively for two and for five equally spaced delta shells. The exact result (3.49) is indicated in the figures by a dashed line. For the spacings we used $\frac{1}{2}d, 1\frac{1}{2}d, 2\frac{1}{2}d, \dots, (N - \frac{1}{2})d$, where $d = a/N$ and N the number of shells. For all measures we took d .

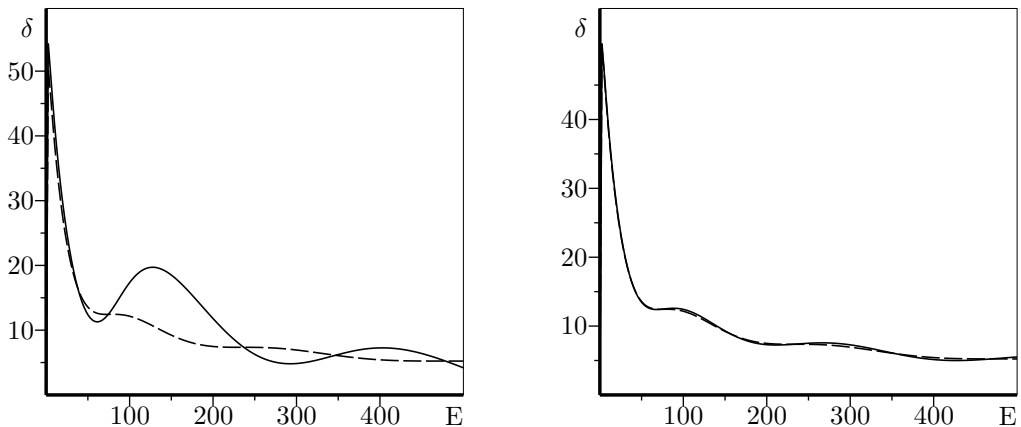


Figure 3.6: Phase shifts for 2 delta shells (lefthand side picture) and for 5 delta shells (righthand side picture). The shells are distributed equally spaced over the width, a , of the well (see text). The intensity of each shell is given by $aV_0/2$ and $aV_0/5$ respectively. For the depth, V_0 , and the width, a , of the well we have chosen here the same values, *i.e.* -8 and 0.5 respectively, as for the results depicted in figure (3.1). The dashed line is the exact solution for the spherical well.

Notice from figure (3.6) that the approximation is already rather good for five delta shells.

The wave functions can be calculated as follows. First, we define the pairs of coefficients A_i and B_i which determine the wave function in the i -th interval, according to

$$u(r) = A_i \sin(kr) + B_i \left(-\frac{\cos(kr)}{k} \right) \quad \text{for } r \in [b_i, b_{i+1}] \quad , \quad (3.83)$$

In the zeroth interval one has $b_0 = 0$ and moreover, from relation (3.68),

$$A_0 = A \quad \text{and} \quad B_0 = 0 \quad . \quad (3.84)$$

Furthermore, we consider $b_{N+1} \rightarrow \infty$.

For the other intervals, by the definition given in formula (3.79), one has the relations

$$\begin{pmatrix} A_i \\ B_i \end{pmatrix} = X(b_i, \Delta_i) \begin{pmatrix} A_{i-1} \\ B_{i-1} \end{pmatrix} . \quad (3.85)$$

With the help of relation (3.85) one can calculate all coefficients in all intervals, hence determine the wave function. An example has been depicted in figure (3.7).

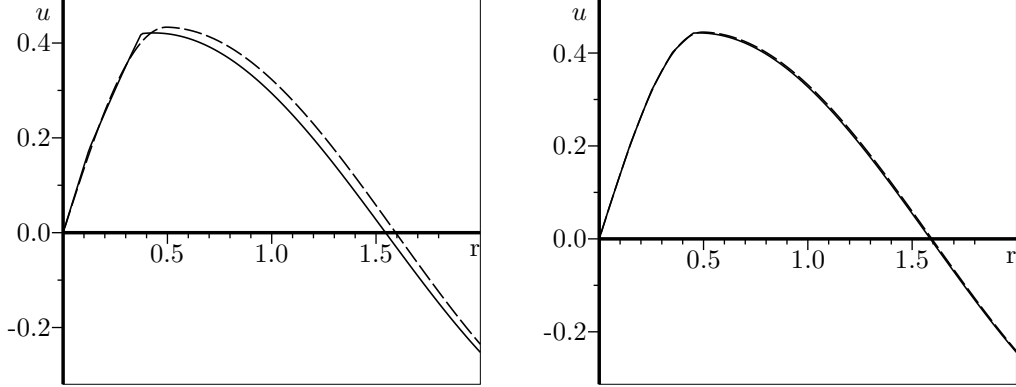


Figure 3.7: Wave function for 2 and for 5 delta shells at $E = 2$. The shells are distributed equally spaced over the *well width* a . The coupling of each shell is given by $aV_0/2$. The dashed line is the exact solution for the spherical well ($V_0 = -8.0$ and $a = 0.5$).

3.7.5 Detailed study of the delta-shell approximation

Let us assume that we dispose over functions $\phi(r)$ and $G(r, r')$ which solve the following equations

$$\left[-\frac{d^2}{dr^2} - E \right] \phi(r) = 0 , \quad \text{and} \quad \left[-\frac{d^2}{dr^2} - E \right] G(r, r') = -\delta(r - r') . \quad (3.86)$$

Then we obtain a formal solution of the wave equation

$$\left(-\frac{d^2}{dr^2} + V(r) - E \right) u(r) = 0 , \quad (3.87)$$

by the expression

$$u(r) = \phi(r) + \int_0^\infty dr' G(r, r') V(r') u(r') . \quad (3.88)$$

This can most conveniently be seen, using formulas (3.86) and (3.88), by performing

$$\begin{aligned} \left(-\frac{d^2}{dr^2} - E \right) u(r) &= \left(-\frac{d^2}{dr^2} - E \right) \left\{ \phi(r) + \int_0^\infty dr' G(r, r') V(r') u(r') \right\} \\ &= 0 + \int_0^\infty dr' [-\delta(r - r')] V(r') u(r') = -V(r) u(r) \end{aligned} \quad (3.89)$$

which leads exactly to equation (3.87).

Now, the integral in equation (3.88) can be approximated by a sum

$$u(r) = \phi(r) + \sum_{n=0}^{\infty} \Delta_n G(r, r_n) V(r_n) u(r_n) \quad , \quad (3.90)$$

where $0 < r_1 < r_2 < \dots$ and where $\Delta_1, \Delta_2, \dots$ represent the measures which belong to the distribution $\{r_n\}$.

For a short-range potential the summation in formula (3.90) can moreover be truncated. We obtain then

$$u(r) = \phi(r) + \sum_{n=0}^N \Delta_n G(r, r_n) V(r_n) u(r_n) \quad . \quad (3.91)$$

This can again be written in the form of an integral equation, as follows

$$u(r) = \phi(r) + \int_0^{\infty} dr' G(r, r') \sum_{n=0}^N \Delta_n V(r_n) \delta(r' - r_n) u(r') \quad . \quad (3.92)$$

Hence, when we define

$$U(r) = \sum_{n=0}^N \Delta_n V(r_n) \delta(r - r_n) \quad , \quad (3.93)$$

then wave function (3.92) solves the wave equation (3.87) with $V(r)$ substituted by $U(r)$. The resulting equation can be solved by the method that we have exposed in the previous paragraphs.

3.7.6 A closer look at the X -matrices

Let us inspect here in more detail the X -matrices which are defined in formula (3.79). For that purpose we define two linearly independent solutions, F and G , of equation (3.60) for $r \neq b$, by

$$F(r) = \sin(kr) \quad \text{and} \quad G(r) = -\frac{\cos(kr)}{k} \quad , \quad (3.94)$$

Notice that those functions have been defined such that their Wronskian has the following property

$$\begin{aligned} W(F, G)(r) &= F(r)G'(r) - F'(r)G(r) \\ &= \sin(kr) \sin(kr) - (k \cos(kr)) \left(-\frac{\cos(kr)}{k} \right) = 1 \\ \text{and} & \end{aligned} \quad (3.95)$$

$$\begin{aligned} W(G, F)(r) &= G(r)F'(r) - G'(r)F(r) \\ &= \sin(kr) \sin(kr) - \left(-\frac{\cos(kr)}{k} \right) (k \cos(kr)) = 1 \quad . \end{aligned}$$

For formula (3.67) we obtain then

$$\begin{pmatrix} u(r) \\ u'(r) \end{pmatrix} = \begin{pmatrix} F(r) & G(r) \\ F'(r) & G'(r) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}, \quad (3.96)$$

with C and D as defined in formula (3.68). Whereas, for the propagator (3.71) we find

$$\mathcal{G}(r_2, r_1) = \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \begin{pmatrix} G'(r_1) & -G(r_1) \\ -F'(r_1) & F(r_1) \end{pmatrix}. \quad (3.97)$$

Using formulas (3.95), (3.96) and (3.97), we verify, for the case that there is no delta-shell in the interval $[r_1, r_2]$, that

$$\begin{aligned} \mathcal{G}(r_2, r_1) \begin{pmatrix} u(r_1) \\ u'(r_1) \end{pmatrix} &= \\ &= \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \begin{pmatrix} G'(r_1) & -G(r_1) \\ -F'(r_1) & F(r_1) \end{pmatrix} \begin{pmatrix} F(r_1) & G(r_1) \\ F'(r_1) & G'(r_1) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\ &= \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \times \\ &\quad \times \begin{pmatrix} G'(r_1)F(r_1) - G(r_1)F'(r_1) & G'(r_1)G(r_1) - G(r_1)G'(r_1) \\ -F'(r_1)F(r_1) + F(r_1)F'(r_1) & -F'(r_1)G(r_1) + F(r_1)G'(r_1) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\ &= \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} u(r_2) \\ u'(r_2) \end{pmatrix}, \quad (3.98) \end{aligned}$$

which confirms formulas (3.69) and (3.71). Whereas for the case that there is only one delta-shell, at $r = b$, in the interval $[r_1, r_2]$, we obtain, by also using formula (3.73), the following result

$$\begin{aligned} \mathcal{G}(r_2, r \downarrow b) \begin{pmatrix} 1 & 0 \\ aV_0 & 1 \end{pmatrix} \mathcal{G}(r \uparrow b, r_1) \begin{pmatrix} u(r_1) \\ u'(r_1) \end{pmatrix} &= \\ &= \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \begin{pmatrix} G'(b) & -G(b) \\ -F'(b) & F(b) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ aV_0 & 1 \end{pmatrix} \times \\ &\quad \times \begin{pmatrix} F(b) & G(b) \\ F'(b) & G'(b) \end{pmatrix} \begin{pmatrix} G'(r_1) & -G(r_1) \\ -F'(r_1) & F(r_1) \end{pmatrix} \begin{pmatrix} F(r_1) & G(r_1) \\ F'(r_1) & G'(r_1) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\ &= \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \times \end{aligned}$$

$$\begin{aligned}
& \times \begin{pmatrix} G'(b)F(b) - G(b)aV_0F(b) + G(b)F'(b) & G'(b)G(b) - G(b)aV_0G(b) - G(b)G'(b) \\ -F'(b)F(b) + F(b)aV_0F(b) + F(b)F'(b) & -F'(b)G(b) + F(b)aV_0G(b) + F(b)G'(b) \end{pmatrix} \times \\
& \quad \times \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\
& = \begin{pmatrix} F(r_2) & G(r_2) \\ F'(r_2) & G'(r_2) \end{pmatrix} \begin{pmatrix} 1 - G(b)aV_0F(b) & -G(b)aV_0G(b) \\ F(b)aV_0F(b) & 1 + F(b)aV_0G(b) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \quad .(3.99)
\end{aligned}$$

Notice that the central matrix, given by

$$X(b, a) = \begin{pmatrix} 1 - G(b)aV_0F(b) & -G(b)aV_0G(b) \\ F(b)aV_0F(b) & 1 + F(b)aV_0G(b) \end{pmatrix} . \quad (3.100)$$

does not contain derivatives of the functions defined in formula (3.94).

Chapter 4

Formal scattering theory

In chapter (3) we discussed the dispersion of a wave packet from a target which is placed at the origin of our coordinate system. In particular, we constructed a solution of the time development operator H which at the instant of time $t = 0$ describes a wave packet concentrated at the macroscopical distance r_0 away from and moving towards the scatterer. At much later times this solution describes then a spherically expanding wave pulse which passes through the detectors, placed at macroscopic distances also of the order of r_0 away from the target.

Here, we will follow a slightly different strategy. As in chapter (3), we concentrate on elastic nonresonant scattering from a target situated at the origin of the coordinate system. However, now we will concentrate on a single projectile particle. An incoming projectile particle is characterized by its momentum, \vec{k}_{in} , long before scattering ($t \downarrow -\infty$), whereas an outgoing projectile particle is characterized by its momentum, \vec{k}_{out} , a long time after scattering ($t \uparrow +\infty$). Notice that, since we deal with elastic scattering, the energy of the projectile particle is unchanged by the scattering process, which implies

$$\left(\vec{k}_{\text{in}}\right)^2 = \left(\vec{k}_{\text{out}}\right)^2 = k^2 \quad . \quad (4.1)$$

We will moreover assume here that the projectile particle enters the interaction region some time before $t = 0$ and leaves the interaction region some time after $t = 0$.

The time development of the wave function $\psi(\vec{r}, t)$ is assumed to be described by a Hamiltonian of the form

$$H = H_0 + V \quad , \quad (4.2)$$

where the potential V is supposed to represent the interaction of the projectile particle with the target and thus of short range, whereas H_0 describes the time development of the projectile particle outside the interaction region. Throughout these notes we will always assume that H_0 is simply the kinetic energy operator as in the Hamiltonian (3.2) and V as given in formula (3.3). But in more sophisticated applications H_0 may include part of the interaction, provided that the solutions to the eigenvalue problem $H_0\Psi = E\Psi$ are known.

In the following we wish to work in the momentum representation, for which the time independent basis states are denoted by $|\vec{k}\rangle$, and which is associated to the coordinate representation, for which the time independent basis states are denoted by $|\vec{r}\rangle$, by the following relation

$$\langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} \quad , \quad (4.3)$$

representing the plane wave approximation of a freely moving wave packet. When H_0 is just given by the kinetic term of equation (3.2), then one has in the momentum representation the equation

$$H_0 | \vec{k} \rangle = E(k) | \vec{k} \rangle \quad \text{where} \quad E(k) = \frac{k^2}{2m} \quad . \quad (4.4)$$

which, comparing to formula (3.33), implies that we may identify

$$\langle \vec{r} | \vec{k} \rangle = \phi(\vec{k}, \vec{r}) \quad . \quad (4.5)$$

4.1 The Møller operators

When a system is described by a wave equation of the form

$$i \frac{\partial}{\partial t} \chi(\vec{r}, t) = \mathcal{H} \chi(\vec{r}, t) \quad , \quad (4.6)$$

then its time evolution is given by

$$\chi(\vec{r}, t) = e^{-i\mathcal{H}t} \chi(\vec{r}, t=0) \quad , \quad (4.7)$$

for any arbitrary initial wave function $\chi(\vec{r}, 0)$. This, because the wave function (4.7) satisfies the wave equation (4.6), as can easily be seen from

$$i \frac{\partial}{\partial t} \chi(\vec{r}, t) = i(-i\mathcal{H}) e^{-i\mathcal{H}t} \chi(\vec{r}, 0) = \mathcal{H} \chi(\vec{r}, t) \quad , \quad (4.8)$$

independent of the choice for $\chi(\vec{r}, 0)$.

When we apply the above to the time development operators H_0 and H , defined in formula (4.2), for which we denote their solutions by ϕ and ψ respectively, then we have the following solutions to the respective wave equations

$$\phi(\vec{r}, t) = e^{-iH_0 t} \phi(\vec{r}, 0) \quad \text{and} \quad \psi(\vec{r}, t) = e^{-iH t} \psi(\vec{r}, 0) \quad , \quad (4.9)$$

for arbitrary initial wave functions $\phi(\vec{r}, 0)$ and $\psi(\vec{r}, 0)$.

Now, since in the limit $t \downarrow -\infty$ the time development operators H_0 and H are supposed to be equal, we may expect that there exist solutions to their respective wave equations which in the same limit are equal, and similar for the limit $t \uparrow +\infty$. Consequently, we assume that there exists a solution $\phi_i(\vec{r}, t)$ of the wave equation related to H_0 which in the limit $t \downarrow -\infty$ equals a solution $\psi_i(\vec{r}, t)$ of the wave equation related to H , and similarly $\phi_f(\vec{r}, t)$ and $\psi_f(\vec{r}, t)$ in the limit $t \uparrow +\infty$, *i.e.*

$$\begin{aligned} \lim_{t \downarrow -\infty} \{ \psi_i(\vec{r}, t) - \phi_i(\vec{r}, t) \} &= 0 \quad , \\ \text{and} & \\ \lim_{t \uparrow +\infty} \{ \psi_f(\vec{r}, t) - \phi_f(\vec{r}, t) \} &= 0 \quad . \end{aligned} \quad (4.10)$$

By the use of the expressions of formula (4.9) for the time development of respectively ϕ and ψ , the above formulas (4.10) turn into

$$\begin{aligned} \lim_{t \downarrow -\infty} \left\{ e^{-iHt} \psi_i(\vec{r}, 0) - e^{-iH_0 t} \phi_i(\vec{r}, 0) \right\} &= 0 \quad , \\ \text{and} & \\ \lim_{t \uparrow +\infty} \left\{ e^{-iHt} \psi_f(\vec{r}, 0) - e^{-iH_0 t} \phi_f(\vec{r}, 0) \right\} &= 0 \quad , \end{aligned} \tag{4.11}$$

which relations, upon multiplying by $\exp(iHt)$ from the left, give the following equations

$$\begin{aligned} \psi_i(\vec{r}, 0) &= \lim_{t \downarrow -\infty} e^{iHt} e^{-iH_0 t} \phi_i(\vec{r}, 0) \\ \text{and} & \\ \psi_f(\vec{r}, 0) &= \lim_{t \uparrow +\infty} e^{iHt} e^{-iH_0 t} \phi_f(\vec{r}, 0) \quad . \end{aligned} \tag{4.12}$$

At this stage it is convenient to introduce the Møller operators, defined by

$$\Omega^{(+)} = \lim_{t \downarrow -\infty} e^{iHt} e^{-iH_0 t} \quad \text{and} \quad \Omega^{(-)} = \lim_{t \uparrow +\infty} e^{iHt} e^{-iH_0 t} \quad . \tag{4.13}$$

After which definition we obtain for formula (4.12) the expressions

$$\psi_i(\vec{r}, 0) = \Omega^{(+)} \phi_i(\vec{r}, 0) \quad \text{and} \quad \psi_f(\vec{r}, 0) = \Omega^{(-)} \phi_f(\vec{r}, 0) \quad . \tag{4.14}$$

For the Møller operators one has the following property

$$H \Omega^{(\pm)} = \Omega^{(\pm)} H_0 \quad , \tag{4.15}$$

which we will proof below for $\Omega^{(+)}$:

When, in general, a function of the time t tends to zero in the limit $t \downarrow -\infty$, then its derivatimes with respect to t also vanish in the same limit, hence for the first expression in formula (4.11) one has

$$\begin{aligned} 0 &= \lim_{t \downarrow -\infty} \left[i \frac{\partial}{\partial t} \left\{ e^{-iHt} \psi_i(\vec{r}, 0) - e^{-iH_0 t} \phi_i(\vec{r}, 0) \right\} \right] \\ &= \lim_{t \downarrow -\infty} \left\{ e^{-iHt} H \psi_i(\vec{r}, 0) - e^{-iH_0 t} H_0 \phi_i(\vec{r}, 0) \right\} \quad , \end{aligned}$$

which relation, upon multiplying by $\exp(iHt)$ from the left, gives the following equation

$$H \psi_i(\vec{r}, 0) = \lim_{t \downarrow -\infty} e^{iHt} e^{-iH_0 t} H_0 \phi_i(\vec{r}, 0) \quad .$$

Substitution of formulas (4.13) and (4.14) leads to

$$H \Omega^{(+)} \phi_i(\vec{r}, 0) = \Omega^{(+)} H_0 \phi_i(\vec{r}, 0) \quad ,$$

which proves formula (4.15) for $\Omega^{(+)}$, since the result is valid for an arbitrary state ϕ_i . For the other Møller operator, $\Omega^{(-)}$, the proof is similar because of formula (4.11).

The property (4.15) for the Møller operators has the following interesting consequence:

The eigenstates $|\vec{k}\rangle$ of the Hamiltonian H_0 , as defined in formula (4.4), represent freely moving particles with a well defined momentum \vec{k} . Now, because of momentum conservation, when a freely moving particle has momentum \vec{k} at the instant of time $t = 0$, then it has momentum \vec{k} for all times. Hence, the wave function

$$e^{-iH_0t} |\vec{k}\rangle$$

describes a freely moving particle with a definite momentum equal to \vec{k} . Consequently, from their definition in formula (4.12) one has that the wave functions

$$|\psi^{(\pm)}(\vec{k})\rangle = \Omega^{(\pm)} |\vec{k}\rangle \quad (4.16)$$

are states which at $t \rightarrow \pm\infty$ coincide with a particle of definite momentum \vec{k} . Moreover, because of the property (4.15), also using the eigenstate equation (4.4), one finds that the wave functions (4.16) are eigenstates of the scattering Hamiltonian H , as

$$H |\psi^{(\pm)}(\vec{k})\rangle = H \Omega^{(\pm)} |\vec{k}\rangle = \Omega^{(\pm)} H_0 |\vec{k}\rangle = \Omega^{(\pm)} E(k) |\vec{k}\rangle = E(k) |\psi^{(\pm)}(\vec{k})\rangle . \quad (4.17)$$

Now, since a particle enters the interaction region with momentum \vec{k}_{in} and leaves it with momentum \vec{k}_{out} , following their definition in formula (4.16), during interaction its state is changed

$$\text{from } |\psi^{(+)}(\vec{k}_{\text{in}})\rangle \text{ to } |\psi^{(-)}(\vec{k}_{\text{out}})\rangle , \quad (4.18)$$

where $|\psi^{(+)}(\vec{k}_{\text{in}})\rangle$ and $|\psi^{(-)}(\vec{k}_{\text{out}})\rangle$ describe respectively an incoming projectile particle with momentum \vec{k}_{in} and an outgoing projectile particle with momentum \vec{k}_{out} .

4.2 The scattering operator S

The matrix elements $S(\vec{k}_{\text{out}}, \vec{k}_{\text{in}})$ of the scattering operator S give the probability that a projectile particle, which enters the interaction region with momentum \vec{k}_{in} , leaves this region with momentum \vec{k}_{out} . By virtue of the definitions expressed in formula (4.18), such transition probabilities are given by

$$S(\vec{k}_{\text{out}}, \vec{k}_{\text{in}}) = \langle \psi^{(-)}(\vec{k}_{\text{out}}) | \psi^{(+)}(\vec{k}_{\text{in}}) \rangle . \quad (4.19)$$

Substitution of the definition given in formula (4.16), gives moreover

$$S(\vec{k}_{\text{out}}, \vec{k}_{\text{in}}) = \langle \vec{k}_{\text{out}} | [\Omega^{(-)}]^\dagger \Omega^{(+)} | \vec{k}_{\text{in}} \rangle . \quad (4.20)$$

Now, since $|\vec{k}_{\text{in}}\rangle$ and $|\vec{k}_{\text{out}}\rangle$ are both supposed to represent arbitrary elements of an orthonormal basis of eigenstates of H_0 , we may define

$$S = [\Omega^{(-)}]^\dagger \Omega^{(+)} . \quad (4.21)$$

The set of states $|\psi^{(-)}(\vec{k})\rangle$ forms a complete basis of eigenstates of the Hamiltonian H , and so does the set of states $|\psi^{(+)}(\vec{k})\rangle$. That they are eigenstates of H can be seen from formula (4.17), whereas their normalizations are given by

$$\langle \psi^{(\pm)}(\vec{k}') | \psi^{(\pm)}(\vec{k}) \rangle = \langle \vec{k}' | [\Omega^{(\pm)}]^\dagger \Omega^{(\pm)} | \vec{k} \rangle = \langle \vec{k}' | \vec{k} \rangle = \delta^{(3)}(\vec{k}' - \vec{k}) , \quad (4.22)$$

because the Møller operators are unitary as can easily be seen from their definition in formula (4.13).

Any solution of the stationary wave equation for H can be expanded in either basis. In particular, a state $|\psi^{(+)}(\vec{k})\rangle$, which describes an incoming plane wave long before interaction, can be expanded in the set of basis states $|\psi^{(-)}(\vec{k})\rangle$, which describe outgoing plane waves. Consequently, the matrix elements (4.19) of the S operator are just the corresponding expansion coefficients.

4.3 The Green's operator G_0

The Green's operator or *resolvent*, $G_0(z)$, corresponding to the self-adjoint free Hamiltonian H_0 is defined to be

$$G_0(z) = (z - H_0)^{-1} \quad , \quad (4.23)$$

where z is an arbitrary complex number and where we assumed that the inverse of $(z - H_0)$ exists. Its relation to the retarded Green's function, shown in formula (3.26), is given by

$$G_+(\vec{r}, \vec{r}') = \lim_{\epsilon \downarrow 0} \langle \vec{r} | G_0(E(k) + i\epsilon) | \vec{r}' \rangle \quad . \quad (4.24)$$

Below we will demonstrate that relation (4.24) is correct.

To that aim, we first determine the following nasty integral

$$\lim_{\epsilon \downarrow 0} \int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\vec{k}' \cdot \vec{a}}}{k'^2 - (k^2 + i\epsilon)} \quad . \quad (4.25)$$

We begin by setting up a system of spherical coordinates for the integration variable \vec{k}' , such that the k'_3 -axis coincides with \vec{a} . This then, with ϑ the angle between \vec{k}' and \vec{a} , gives

$$\vec{k}' \cdot \vec{a} = k'a \cos(\vartheta) \quad ,$$

and gives, moreover, for the integral (4.25) the expression

$$\lim_{\epsilon \downarrow 0} \frac{1}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_{-1}^{+1} d \cos(\vartheta) \int_0^\infty k'^2 dk' \frac{e^{ik'a \cos(\vartheta)}}{k'^2 - (k^2 + i\epsilon)} \quad . \quad (4.26)$$

The integrand does not depend on φ , so the related integration yields a factor 2π . For the integral over $\cos(\vartheta)$ we obtain

$$\int_{-1}^{+1} dz e^{ik'az} = \left. \frac{e^{ik'az}}{ik'a} \right|_{-1}^{+1} = \frac{1}{ik'a} \left\{ e^{ik'a} - e^{-ik'a} \right\} \quad ,$$

after which (4.26) turns into

$$\lim_{\epsilon \downarrow 0} \frac{1}{ia(2\pi)^2} \left\{ \int_0^\infty \frac{k' dk' e^{ik'a}}{k'^2 - (k^2 + i\epsilon)} - \int_0^\infty \frac{k' dk' e^{-ik'a}}{k'^2 - (k^2 + i\epsilon)} \right\} \quad . \quad (4.27)$$

When, next, we redefine the integration variable k' in the second term for $-k'$, then the above equation (4.27) takes the form

$$\begin{aligned} \lim_{\epsilon \downarrow 0} \frac{1}{ia(2\pi)^2} \left\{ \int_0^\infty \frac{k' dk' e^{ik'a}}{k'^2 - (k^2 + i\epsilon)} + \int_{-\infty}^0 \frac{k' dk' e^{ik'a}}{k'^2 - (k^2 + i\epsilon)} \right\} = \\ = \lim_{\epsilon \downarrow 0} \frac{1}{ia(2\pi)^2} \int_{-\infty}^{+\infty} \frac{k' dk' e^{ik'a}}{(k' - \sqrt{k^2 + i\epsilon})(k' + \sqrt{k^2 + i\epsilon})} \quad . \quad (4.28) \end{aligned}$$

This integral can be turned into a complex contour integral by closing it, using a half circle with infinite radius in the upper half complex plane. A positive infinite imaginary part for k' in the exponent $\exp(ik'a)$ damps the contribution to the integral of this half circle to zero. The only nonzero contributions for this counterclockwise closed contour come from the residues of the poles in the upper half complex plane. Now, for small ϵ we may approximate

$$\sqrt{k^2 + i\epsilon} \approx k \left(1 + i \frac{\epsilon}{2k^2} \right) .$$

Consequently, the pole at $k = +\sqrt{k^2 + i\epsilon}$ lies in the upper half complex plane and thus gives a contribution to the integral (4.28). Whereas the other pole, at $k = -\sqrt{k^2 + i\epsilon}$, is in the lower half complex plane and hence does not contribute to the integral (4.28). The relevant residue is readily determined and after taking the limit $\epsilon \downarrow 0$, we end up with

$$\frac{2\pi i}{ia(2\pi)^2} e^{ika} = \frac{1}{4\pi} \frac{e^{ika}}{a} \quad (4.29)$$

for the integral (4.25).

After this exercise we return to the retarded Green's function of formula (4.24). We begin by the substitution of the definition of the Green's operator (4.23) in expression (4.24), and moreover apply completeness of the $|\vec{k}\rangle$ -basis by inserting unity, *i.e.*

$$G_+(\vec{r}, \vec{r}') = \lim_{\epsilon \downarrow 0} \int d^3k' \langle \vec{r} | \vec{k}' \rangle \langle \vec{k}' | [E(k) + i\epsilon - H_0]^{-1} | \vec{r}' \rangle .$$

Then we let the Green's operator act to the left, to obtain

$$G_+(\vec{r}, \vec{r}') = \lim_{\epsilon \downarrow 0} \int d^3k' \langle \vec{r} | \vec{k}' \rangle \langle \vec{k}' | [E(k) + i\epsilon - k'^2]^{-1} | \vec{r}' \rangle .$$

Substitution of formulas (4.3) and (4.4) gives moreover

$$G_+(\vec{r}, \vec{r}') = - \left[\lim_{\epsilon \downarrow 0} \int \frac{d^3k'}{(2\pi)^3} \frac{2m e^{i\vec{k}' \cdot (\vec{r} - \vec{r}')}}{k'^2 - (E(k) + i2m\epsilon)} \right] .$$

Comparing this expression with the integral (4.25) and its solution (4.29), we find, after taking $\vec{a} = \vec{r} - \vec{r}'$ and $a = |\vec{r} - \vec{r}'|$, the result

$$G_+(\vec{r}, \vec{r}') = -\frac{m}{2\pi} \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} .$$

which is indeed equal to formula (3.26).

To conclude this section we note that since $[H_0]^\dagger = H_0$, it is easily seen that

$$[G_0(z)]^\dagger = G_0(z^*) . \quad (4.30)$$

4.4 The LS equation in momentum space

In section (3.4) we studied the Lippmann Schwinger equation for the solutions of the stationary Schrödinger equation (3.7). Here, we will rewrite formula (3.32) in the momentum representation. To that aim we define an eigenstate $|\psi^{(+)}(\vec{k})\rangle$ of the Hamiltonian (4.2), *i.e.* to the equation $H\psi = E(k)\psi$, which in coordinate space is related to the solution $\psi^{(+)}(\vec{k}, \vec{r})$ of equation (3.31) by

$$\psi^{(+)}(\vec{k}, \vec{r}) = \langle \vec{r} | \psi^{(+)}(\vec{k}) \rangle . \quad (4.31)$$

Moreover, we define for a local potential V the following relation in the coordinate representation

$$\langle \vec{r} | V | \vec{r}' \rangle = V(\vec{r}) \delta^{(3)}(\vec{r} - \vec{r}') . \quad (4.32)$$

First, we rewrite equation (3.32) to

$$\psi^{(+)}(\vec{k}, \vec{r}) = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} + \int d^3r' \int d^3r'' G_+(\vec{r}, \vec{r}') V(\vec{r}') \delta^{(3)}(\vec{r}' - \vec{r}'') \psi^{(+)}(\vec{k}, \vec{r}'') ,$$

and then we substitute the relations (4.3), (4.24), (4.31), and (4.32), to obtain

$$\langle \vec{r} | \psi^{(+)}(\vec{k}) \rangle = \langle \vec{r} | \vec{k} \rangle + \int d^3r' \int d^3r'' \langle \vec{r} | G_0(E(k) + i\epsilon) | \vec{r}' \rangle \langle \vec{r}' | V | \vec{r}'' \rangle \langle \vec{r}'' | \psi^{(+)}(\vec{k}) \rangle , \quad (4.33)$$

where the limit $\epsilon \downarrow 0$ is implicitly understood. Next we remove two times the identity operation which stems from completeness of the $|\vec{r}\rangle$ -basis, to end up with

$$\langle \vec{r} | \psi^{(+)}(\vec{k}) \rangle = \langle \vec{r} | \vec{k} \rangle + \langle \vec{r} | G_0(E(k) + i\epsilon) V | \psi^{(+)}(\vec{k}) \rangle ,$$

which leads to the following relation

$$|\psi^{(+)}(\vec{k})\rangle = |\vec{k}\rangle + G_0(E(k) + i\epsilon) V |\psi^{(+)}(\vec{k})\rangle . \quad (4.34)$$

This is the Lippmann Schwinger equation in momentum space. Like in the case of the wave function (3.32) for which we wrote the perturbation series (3.35), one may also iterate formula (4.34) in order to obtain (for convenience we write G_0 instead of $G_0(E(k) + i\epsilon)$)

$$\begin{aligned} |\psi^{(+)}(\vec{k})\rangle &= |\vec{k}\rangle + G_0 V |\vec{k}\rangle + G_0 V G_0 V |\vec{k}\rangle + \dots \\ &= |\vec{k}\rangle + \{G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots\} V |\vec{k}\rangle . \end{aligned} \quad (4.35)$$

At this stage it is oportune to define the Green's operator $G(z)$ by

$$G(z) = G_0(z) + G_0(z) V G_0(z) + G_0(z) V G_0(z) V G_0(z) + \dots . \quad (4.36)$$

This series can be summed, using the following expansion for operators A and B :

$$\begin{aligned}
(A - B)^{-1} &= \left(A (1 - A^{-1}B) \right)^{-1} = (1 - A^{-1}B)^{-1} A^{-1} \\
&= \left\{ 1 + A^{-1}B + (A^{-1}B)^2 + (A^{-1}B)^3 + \dots \right\} A^{-1} \\
&= A^{-1} + A^{-1}BA^{-1} + A^{-1}BA^{-1}BA^{-1} + A^{-1}BA^{-1}BA^{-1}BA^{-1} + \dots
\end{aligned} \tag{4.37}$$

So, when we substitute for A the expression $(z - H_0)$, which implies, by formula (4.23), $A^{-1} = G_0(z)$, and for B the potential operator, V , we obtain for the righthand side of formula (4.37) the righthand side of formula (4.36). Consequently, we discover for the Green's operator (4.36) the expression

$$G(z) = (z - H_0 - V)^{-1} = (z - H)^{-1} , \tag{4.38}$$

as a generalization of the definition (4.23), and hence for the series expansion of formula (4.35) the relation

$$\left| \psi^{(+)}(\vec{k}) \right\rangle = \lim_{\epsilon \downarrow 0} [1 + G(E(k) + i\epsilon) V] \left| \vec{k} \right\rangle . \tag{4.39}$$

To conclude this section we note that since $H^\dagger = H$, it is easily seen that

$$[G(z)]^\dagger = G(z^*) . \tag{4.40}$$

4.5 Relation Green's operators and Møller operators

Let $|\phi_0\rangle$ represent an arbitrary state in momentum space, and $|\psi_{\pm}\rangle$ be defined by

$$|\psi_{\pm}\rangle = \Omega^{(\pm)} |\phi_0\rangle = \lim_{t \rightarrow \mp\infty} e^{iHt} e^{-iH_0t} |\phi_0\rangle . \quad (4.41)$$

It is this definition which we would like to rewrite in terms of the Green's operator.

First, we remember to write a function of the time t as the integral of its derivative with respect to t . For $|\psi_{-}\rangle$ we obtain then

$$|\psi_{-}\rangle = \left[e^{iHt} e^{-iH_0t} \right]_{t=0} + \int_0^{+\infty} dt e^{iHt} iV e^{-iH_0t} |\phi_0\rangle ,$$

where the derivative, also using formula (4.2), comes from

$$\frac{\partial}{\partial t} \left\{ e^{iHt} e^{-iH_0t} \right\} = e^{iHt} (iH - iH_0) e^{-iH_0t} = e^{iHt} iV e^{-iH_0t} .$$

So, we arrive for the state $|\psi_{-}\rangle$ of formula (4.41) at the expression

$$|\psi_{-}\rangle = \left\{ 1 + \int_0^{+\infty} dt e^{iHt} iV e^{-iH_0t} \right\} |\phi_0\rangle , \quad (4.42)$$

and similarly for the other state, $|\psi_{+}\rangle$ of formula (4.41), at the expression

$$|\psi_{+}\rangle = \left\{ 1 + \int_{-\infty}^0 dt e^{iHt} iV e^{-iH_0t} \right\} |\phi_0\rangle . \quad (4.43)$$

The integrals of formulas (4.42) and (4.43) are absolutely convergent, in which case one may substitute the integrands for

$$|\psi_{-}\rangle = \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int_0^{+\infty} dt e^{-\epsilon t} e^{iHt} V e^{-iH_0t} \right\} |\phi_0\rangle$$

and

$$|\psi_{+}\rangle = \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int_{-\infty}^0 dt e^{+\epsilon t} e^{iHt} V e^{-iH_0t} \right\} |\phi_0\rangle . \quad (4.44)$$

We can interpret the expressions (4.44) by noting that it differs from the formulas (4.42) and (4.43) by a change in potential from V to $V \exp(-\epsilon|t|)$, which expresses the fact that the motion of any scattering orbit would be unchanged under such redefinition of the potential for small ϵ . This is exactly what one would expect, since we know that the projectile particle eventually moves so far away that the potential ceases to have any effect. The result that one can do scattering theory with V replaced by $V \exp(-\epsilon|t|)$ is known as the *adiabatic theorem*.

When we insert unity, in the form of a complete set of states $|\vec{k}\rangle$, into the equations (4.44), then we find

$$|\psi_{-}\rangle = \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int d^3k \int_0^{+\infty} dt e^{-\epsilon t} e^{iHt} V e^{-iH_0t} |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle$$

and

$$|\psi_{+}\rangle = \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int d^3k \int_{-\infty}^0 dt e^{+\epsilon t} e^{iHt} V e^{-iH_0t} |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle . \quad (4.45)$$

Now, by the property (4.4) we obtain

$$\begin{aligned}
|\psi_{-}\rangle &= \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int d^3 k \int_0^{+\infty} dt e^{-i(E(k) - i\epsilon - H)t} V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle \\
&\text{and} \\
|\psi_{+}\rangle &= \left\{ 1 + i \lim_{\epsilon \downarrow 0} \int d^3 k \int_{-\infty}^0 dt e^{-i(E(k) + i\epsilon - H)t} V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle .
\end{aligned} \tag{4.46}$$

After moreover performing the t integrations, the expressions (4.46) turn into

$$\begin{aligned}
|\psi_{-}\rangle &= \left\{ 1 + \lim_{\epsilon \downarrow 0} \int d^3 k (E(k) - i\epsilon - H)^{-1} V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle \\
&\text{and} \\
|\psi_{+}\rangle &= \left\{ 1 + \lim_{\epsilon \downarrow 0} \int d^3 k (E(k) + i\epsilon - H)^{-1} V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle .
\end{aligned} \tag{4.47}$$

Here, we recognize the Green's operator, $G(E(k) \pm i\epsilon)$, defined in formula (4.38), substitution of which leaves us with

$$\begin{aligned}
|\psi_{-}\rangle &= \left\{ 1 + \lim_{\epsilon \downarrow 0} \int d^3 k G(E(k) - i\epsilon) V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle \\
&\text{and} \\
|\psi_{+}\rangle &= \left\{ 1 + \lim_{\epsilon \downarrow 0} \int d^3 k G(E(k) + i\epsilon) V |\vec{k}\rangle \langle \vec{k}| \right\} |\phi_0\rangle .
\end{aligned} \tag{4.48}$$

Note that the signs of the term $\pm i\epsilon$ correspond to the subscripts \pm of the state vectors ψ_{\pm} , and hence to the superscripts of the operators $\Omega^{(\pm)}$.

Finally, returning to the definitions (4.41), we end up with

$$\Omega^{(\pm)} = 1 + \lim_{\epsilon \downarrow 0} \int d^3 k G(E(k) \pm i\epsilon) V |\vec{k}\rangle \langle \vec{k}| . \tag{4.49}$$

When we apply the above relation (4.49), between Green's and Møller operators, to the case of the states $\psi^{(\pm)}$, which are defined in formula (4.16), then we may perform the \vec{k} -integration, as

$$\begin{aligned}
|\psi^{(\pm)}(\vec{k})\rangle &= \Omega^{(\pm)} |\vec{k}\rangle \\
&= \left\{ 1 + \lim_{\epsilon \downarrow 0} \int d^3 k' G(E(k') \pm i\epsilon) V |\vec{k}'\rangle \langle \vec{k}'| \right\} |\vec{k}\rangle \\
&= |\vec{k}\rangle + \lim_{\epsilon \downarrow 0} \int d^3 k' G(E(k') \pm i\epsilon) V |\vec{k}'\rangle \delta^{(3)}(\vec{k}' - \vec{k}) \\
&= \left\{ 1 + \lim_{\epsilon \downarrow 0} G(E(k) \pm i\epsilon) V \right\} |\vec{k}\rangle .
\end{aligned} \tag{4.50}$$

4.6 The LS equation for the Green's operators

For the Green's operators G_0 , defined in formula (4.23), and G , defined in formula (4.38), we may derive the following Lippmann Schwinger relations.

For the first relation we rewrite formula (4.36) as

$$\begin{aligned} G(z) &= G_0(z) + G_0(z)V \{G_0(z) + G_0(z)VG_0(z) + \dots\} \\ &= G_0(z) + G_0(z)VG(z) \quad . \end{aligned} \tag{4.51}$$

For the second relation we rewrite formula (4.36) as

$$\begin{aligned} G(z) &= G_0(z) + \{G_0(z) + G_0(z)VG_0(z) + \dots\} VG_0(z) \\ &= G_0(z) + G(z)VG_0(z) \quad . \end{aligned} \tag{4.52}$$

Those two equations constitute one of the essential corner stones of the stationary scattering formalism.

4.7 The transition operator T

In scattering theory it is convenient to introduce the transition operator, $T(z)$, which is defined in terms of $G(z)$ and V as

$$T(z) = V + V G(z) V \quad . \quad (4.53)$$

When this expression is multiplied on the left by $G_0(z)$ and moreover relation (4.51) substituted, then we find

$$G_0(z) T(z) = G(z) V \quad . \quad (4.54)$$

Similarly, when expression (4.53) is multiplied on the right by $G_0(z)$ and moreover relation (4.52) substituted, then we find

$$T(z) G_0(z) = V G(z) \quad . \quad (4.55)$$

The most famous Lippmann Schwinger equation is the one for the T operator, which can be obtained by substituting relation (4.54) into the definition (4.53) for the transition operator, since then

$$\mathbf{T}(z) = \mathbf{V} + \mathbf{V} \mathbf{G}_0(z) \mathbf{T}(z) \quad . \quad (4.56)$$

Furthermore, we note that the identity (4.40) for $G(z)$ leads to a corresponding result for $T(z)$, as, assuming that V is Hermitean, is easily seen from formula (4.53) by

$$[T(z)]^\dagger = V + V [G(z)]^\dagger V = V + V G(z^*) V = T(z^*) \quad . \quad (4.57)$$

An other interesting property of $T(z)$ stems from the matrix element

$$\langle \vec{k}' | V | \psi^{(+)}(\vec{k}) \rangle \quad ,$$

which, following formula (4.50) can be casted in the form

$$\lim_{\epsilon \downarrow 0} \langle \vec{k}' | V \{1 + G(E(k) + i\epsilon) V\} | \vec{k} \rangle \quad .$$

Consequently, by the use of the definition (4.53), we then find

$$\langle \vec{k}' | V | \psi^{(+)}(\vec{k}) \rangle = \lim_{\epsilon \downarrow 0} \langle \vec{k}' | T(E(k) + i\epsilon) | \vec{k} \rangle \quad . \quad (4.58)$$

4.8 Relation T and S operators

In order to establish a relation between the transition operator T and the scattering operator S , we start from the definition (4.19)

$$S(\vec{k}', \vec{k}) = \langle \psi^{(-)}(\vec{k}') | \psi^{(+)}(\vec{k}) \rangle . \quad (4.59)$$

To proceed, we determine for $\psi^{(-)}(\vec{k})$, using their definitions (4.16), the following identity

$$|\psi^{(-)}(\vec{k})\rangle - |\psi^{(+)}(\vec{k})\rangle = \Omega^{(-)}|\vec{k}\rangle - \Omega^{(+)}|\vec{k}\rangle ,$$

which by virtue of formula (4.50), equals

$$\lim_{\epsilon \downarrow 0} \{G(E(k) - i\epsilon) - G(E(k) + i\epsilon)\} V |\vec{k}\rangle .$$

So, we find

$$\langle \psi^{(-)}(\vec{k}) | = \langle \psi^{(+)}(\vec{k}) | + \lim_{\epsilon \downarrow 0} \langle \vec{k} | V^\dagger \{G^\dagger(E(k) - i\epsilon) - G^\dagger(E(k) + i\epsilon)\} ,$$

which using the property (4.40), moreover assuming that the potential V is Hermitean, can be written as

$$\langle \psi^{(-)}(\vec{k}) | = \langle \psi^{(+)}(\vec{k}) | + \lim_{\epsilon \downarrow 0} \langle \vec{k} | V \{G(E(k) + i\epsilon) - G(E(k) - i\epsilon)\} .$$

This expression substituted in formula (4.59) gives

$$S(\vec{k}', \vec{k}) = \quad (4.60)$$

$$\langle \psi^{(+)}(\vec{k}') | \psi^{(+)}(\vec{k}) \rangle + \lim_{\epsilon \downarrow 0} \langle \vec{k}' | V \{G(E(k') + i\epsilon) - G(E(k') - i\epsilon)\} | \psi^{(+)}(\vec{k}) \rangle .$$

The first term on the righthand side of equation (4.60) is handled by formula (4.22). Using the definition of the Green's operator (4.38), we find for the second term on the righthand side of equation (4.60) the following

$$\langle \vec{k}' | V \{(E(k') + i\epsilon - H)^{-1} - (E(k') - i\epsilon - H)^{-1}\} | \psi^{(+)}(\vec{k}) \rangle ,$$

which, because of relation (4.17), turns into

$$\begin{aligned} & \langle \vec{k}' | V \{(E(k') + i\epsilon - E(k))^{-1} - (E(k') - i\epsilon - E(k))^{-1}\} | \psi^{(+)}(\vec{k}) \rangle = \\ & = \{(E(k') + i\epsilon - E(k))^{-1} - (E(k') - i\epsilon - E(k))^{-1}\} \langle \vec{k}' | V | \psi^{(+)}(\vec{k}) \rangle . \end{aligned}$$

Next, we use the following representation of the Dirac delta function:

$$2\pi i \delta(x) = \lim_{\epsilon \rightarrow 0} \frac{2i\epsilon}{x^2 + \epsilon^2} = \lim_{\epsilon \rightarrow 0} \left\{ \frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon} \right\} ,$$

which when substituted in our final expression, gives

$$-2\pi i \delta(E(k') - E(k)) \langle \vec{k}' | V | \psi^{(+)}(\vec{k}) \rangle . \quad (4.61)$$

Inserting the results (4.22) and (4.61) into equation (4.60), leads to

$$S(\vec{k}', \vec{k}) = \delta^{(3)}(\vec{k}' - \vec{k}) - 2\pi i \delta(E(k') - E(k)) \langle \vec{k}' | V | \psi^{(+)}(\vec{k}) \rangle . \quad (4.62)$$

Here, we may moreover substitute relation (4.58) for the transition operator, to end up for (4.62) with

$$S(\vec{k}', \vec{k}) = \delta^{(3)}(\vec{k}' - \vec{k}) - 2\pi i \delta(E(k') - E(k)) \langle \vec{k}' | T(E(k) + i\epsilon) | \vec{k} \rangle . \quad (4.63)$$

This is one of the central results of time-independent scattering theory.

Formula (4.63) shows explicitly that the matrix elements of the S operator vanish when $E(k')$ does not equal $E(k)$, even when the matrix elements of the T operator do not vanish in that case. In other words, the matrix elements of S are *on-shell*, whereas the matrix elements of T might be *off-shell*.

Chapter 5

Examples

In this chapter we will work out in some detail two examples of models for the description of scattering by means of a potential in Schrödinger theory.

5.1 The potential term

The potential term in the configuration space wave equation takes in general the form

$$\int d^3r' V(\vec{r}, \vec{r}') \psi(\vec{r}') \quad , \quad (5.1)$$

which gives then the wave equation

$$-\frac{1}{2\mu} \nabla_r^2 \psi(\vec{r}) + \int d^3r' V(\vec{r}, \vec{r}') \psi(\vec{r}') = E \psi(\vec{r}) \quad , \quad (5.2)$$

where E represents the total energy of the system.

In momentum space we define

$$V(\vec{k}, \vec{k}') = \int \frac{d^3r}{(2\pi)^{3/2}} e^{-i\vec{k} \cdot \vec{r}} \int \frac{d^3r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}, \vec{r}') \quad , \quad (5.3)$$

for which quantity we may study the following expression

$$\begin{aligned} & \int \frac{d^3k''}{(2\pi)^{3/2}} e^{i\vec{k}'' \cdot \vec{r}} \int d^3k' V(\vec{k}'', \vec{k}') \phi(\vec{k}') = \\ &= \int \frac{d^3k''}{(2\pi)^{3/2}} e^{i\vec{k}'' \cdot \vec{r}} \int d^3k' \int \frac{d^3r''}{(2\pi)^{3/2}} e^{-i\vec{k}'' \cdot \vec{r}''} \int \frac{d^3r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}'', \vec{r}') \phi(\vec{k}') \\ &= \int d^3k' \int \frac{d^3r''}{(2\pi)^{3/2}} \left[\int \frac{d^3k''}{(2\pi)^{3/2}} e^{i\vec{k}'' \cdot (\vec{r} - \vec{r}'')} \right] \int \frac{d^3r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}'', \vec{r}') \phi(\vec{k}') \\ &= \int d^3k' \int \frac{d^3r''}{(2\pi)^{3/2}} (2\pi)^{3/2} \delta^{(3)}(\vec{r} - \vec{r}'') \int \frac{d^3r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}'', \vec{r}') \phi(\vec{k}') \\ &= \int d^3r' V(\vec{r}, \vec{r}') \int \frac{d^3k'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} \phi(\vec{k}') \end{aligned}$$

$$= \int d^3 r' V(\vec{r}, \vec{r}') \psi(\vec{r}') \quad . \quad (5.4)$$

The result (5.4) may be substituted in the configuration space wave equation (5.2), to give

$$\begin{aligned} & \int \frac{d^3 k}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{r}} \frac{1}{2\mu} k^2 \phi(\vec{k}) + \int \frac{d^3 k}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{r}} \int d^3 k' V(\vec{k}, \vec{k}') \phi(\vec{k}') = \\ & = E \int \frac{d^3 k}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{r}} \phi(\vec{k}) \quad , \end{aligned} \quad (5.5)$$

or also

$$\int \frac{d^3 k}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{r}} \left\{ \left(\frac{k^2}{2\mu} - E \right) \phi(\vec{k}) + \int d^3 k' V(\vec{k}, \vec{k}') \phi(\vec{k}') \right\} = 0 \quad , \quad (5.6)$$

which gives for the wave equation in momentum space the expression

$$\frac{k^2}{2\mu} \phi(\vec{k}) + \int d^3 k' V(\vec{k}, \vec{k}') \phi(\vec{k}') = E \phi(\vec{k}) \quad . \quad (5.7)$$

5.1.1 Local potentials

For a local potential in the configuration space wave equation (5.2) one may select the following general form

$$V(\vec{r}, \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}') V(\vec{r}') \quad , \quad (5.8)$$

since indeed

$$\begin{aligned} & \int d^3 r' V(\vec{r}, \vec{r}') \psi(\vec{r}') = \int d^3 r' \delta^{(3)}(\vec{r} - \vec{r}') V(\vec{r}') \psi(\vec{r}') = \\ & = \int dr' \delta(r - r') \int d\vartheta' \delta(\vartheta - \vartheta') \int d\varphi' \delta(\varphi - \varphi') V(r', \vartheta', \varphi') \psi(r', \vartheta', \varphi') \\ & = V(r, \vartheta, \varphi) \psi(r, \vartheta, \varphi) = V(\vec{r}) \psi(\vec{r}) \quad . \end{aligned} \quad (5.9)$$

The momentum space analogon of the configuration space potential is defined in formula (5.3), which, when applied to expression (5.8), gives

$$\begin{aligned} V(\vec{k}, \vec{k}') & = \int \frac{d^3 r}{(2\pi)^{3/2}} e^{-i\vec{k} \cdot \vec{r}} \int \frac{d^3 r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}, \vec{r}') \\ & = \int \frac{d^3 r}{(2\pi)^{3/2}} e^{-i\vec{k} \cdot \vec{r}} \int \frac{d^3 r'}{(2\pi)^{3/2}} e^{i\vec{k}' \cdot \vec{r}'} \delta^{(3)}(\vec{r} - \vec{r}') V(\vec{r}') \\ & = \int \frac{d^3 r}{(2\pi)^3} e^{i(-\vec{k} + \vec{k}') \cdot \vec{r}} V(\vec{r}) \quad . \end{aligned} \quad (5.10)$$

5.1.2 Spherically symmetric local potentials

For spherically symmetric local potentials in configuration space, of the form

$$V(\vec{r}, \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}') V(r) \quad , \quad (5.11)$$

one may moreover perform the angular integrations of formula (5.10), to obtain for the momentum space potential the following

$$\begin{aligned} V(\vec{k}, \vec{k}') &= (2\pi)^{-3} \int_0^\infty r^2 dr V(r) \int_0^{2\pi} d\varphi \int_{-1}^{+1} d \cos(\vartheta) e^{i \left| -\vec{k} + \vec{k}' \right| r \cos(\vartheta)} \\ &= \frac{1}{2\pi^2} \int_0^\infty r^2 dr V(r) j_0 \left(\left| -\vec{k} + \vec{k}' \right| r \right) \end{aligned} \quad (5.12)$$

In the book [2] of Morse and Feshbach, in chapter 11 at page 1574, we find furthermore the following expansion for the spherical Bessel function

$$j_0 \left(r \sqrt{k^2 + k'^2 - 2\vec{k} \cdot \vec{k}'} \right) = \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{k} \cdot \hat{k}') j_\ell(kr) j_\ell(k'r) \quad , \quad (5.13)$$

which leads for (5.12) to

$$V(\vec{k}, \vec{k}') = \frac{1}{2\pi^2} \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{k} \cdot \hat{k}') \int_0^\infty r^2 dr V(r) j_\ell(kr) j_\ell(k'r) \quad . \quad (5.14)$$

5.2 Relation transition amplitude and T -matrix

The relation between the transition amplitude and the retarded wave functions is given in formula (3.39), *i.e.*

$$f(\vec{k}, \hat{r}) = -\sqrt{2\pi} \mu \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} V(\vec{r}') \psi^{(+)}(\vec{k}, \vec{r}') \quad . \quad (5.15)$$

In ket-notation and for a local potential one has

$$\begin{aligned} f(\vec{k}, \hat{r}) &= -\sqrt{2\pi} \mu \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} \int d^3 r'' V(\vec{r}'') \delta^{(3)}(\vec{r}' - \vec{r}'') \psi^{(+)}(\vec{k}, \vec{r}'') \\ &= -\sqrt{2\pi} \mu \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} \int d^3 r'' \langle \vec{r}' | V | \vec{r}'' \rangle \langle \vec{r}'' | \Omega^+ | \vec{k} \rangle \\ &= -\sqrt{2\pi} \mu \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} \langle \vec{r}' | V \Omega^+ | \vec{k} \rangle \quad , \end{aligned} \quad (5.16)$$

where we also introduced the Møller operator Ω^+ , defined in formula (4.13). Next, we use formulas (4.3), (4.50) and (4.58) to obtain the result

$$\begin{aligned} f(\vec{k}, \hat{r}) &= -\sqrt{2\pi} \mu \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} \int d^3 k' \langle \vec{r}' | \vec{k}' \rangle \langle \vec{k}' | V \Omega^+ | \vec{k} \rangle \\ &= -\sqrt{2\pi} \mu \int d^3 k' \left\{ \int d^3 r' e^{-ik\hat{r} \cdot \vec{r}'} \frac{e^{i\vec{k}' \cdot \vec{r}'}}{(2\pi)^{3/2}} \right\} \langle \vec{k}' | V \Omega^+ | \vec{k} \rangle \\ &= -\frac{\mu}{2\pi} \int d^3 k' \left\{ \int d^3 r' e^{i(\vec{k}' - k\hat{r}) \cdot \vec{r}'} \right\} \langle \vec{k}' | T(k^2 + i\epsilon) | \vec{k} \rangle \quad , \end{aligned} \quad (5.17)$$

The integration in configuration space can, by the use of formula (19.68) of [1], be handled as follows

$$\begin{aligned} \int d^3 r' e^{i(\vec{k}' - k\hat{r}) \cdot \vec{r}'} &= (2\pi)^3 \delta^{(3)}(\vec{k}' - k\hat{r}) \\ &= 2\pi^2 \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{r} \cdot \hat{k}') \frac{\delta(k - k')}{k^2} \quad . \end{aligned} \quad (5.18)$$

So, after calculating the matrix elements of the T -operator, one still has to perform integrations.

Now, let us assume that the matrix elements of T have the following genuine form in the case of spherical symmetry

$$\langle \vec{k} | T(k^2 + i\epsilon) | \vec{k}' \rangle = \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{k}') T_{\ell}(k, k') \quad . \quad (5.19)$$

When we substitute both expansions (5.19) and (5.18) into formula (5.17), then we find

$$\begin{aligned}
f(\vec{k}, \hat{r}) &= \tag{5.20} \\
&= -\pi\mu \sum_{\ell, \ell'=0}^{\infty} (2\ell+1)(2\ell'+1) \int d^3k' P_{\ell}(\hat{k} \cdot \hat{k}') T_{\ell}(k, k') P_{\ell'}(\hat{r} \cdot \hat{k}') \frac{\delta(k-k')}{k^2} .
\end{aligned}$$

Next, let us concentrate on the integration over the angles in k' -space, *i.e.*

$$\int d\Omega_{k'} P_{\ell}(\hat{k} \cdot \hat{k}') P_{\ell'}(\hat{r} \cdot \hat{k}') . \tag{5.21}$$

Here, we may select the z -axis of the \vec{k}' -system in the direction of \vec{k} . But, that does not help much for the second term in the integrand of formula (5.21). However, by the use of the addition theorem (see e.g. formula 9.79 of [1]) we find

$$\begin{aligned}
\int d\Omega_{k'} P_{\ell}(\hat{k} \cdot \hat{k}') P_{\ell'}(\hat{r} \cdot \hat{k}') &= \tag{5.22} \\
&= \int d\Omega_{k'} P_{\ell}(\hat{k} \cdot \hat{k}') \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}(\hat{k} \cdot \hat{r}) Y_{\ell'_z}^{(\ell')}(\hat{k} \cdot \hat{k}') \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}(\hat{k} \cdot \hat{r}) \int d\Omega_{k'} P_{\ell}(\Omega_{k'}) Y_{\ell'_z}^{(\ell')}(\Omega_{k'}) .
\end{aligned}$$

Then, we substitute for $P_{\ell}(\Omega_{k'})$ in the above expression (5.22) formulas (9.78) and (9.65a) of [1], to find

$$\begin{aligned}
\int d\Omega_{k'} P_{\ell}(\hat{k} \cdot \hat{k}') P_{\ell'}(\hat{r} \cdot \hat{k}') &= \tag{5.23} \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}(\hat{k} \cdot \hat{r}) \int d\Omega_{k'} \sqrt{\frac{4\pi}{2\ell+1}} Y_0^{(\ell)*}(\Omega_{k'}) Y_{\ell'_z}^{(\ell')}(\Omega_{k'}) ,
\end{aligned}$$

which, after applying the orthogonality of spherical harmonics (see e.g. [1] formula 9.69), leads to

$$\begin{aligned}
\int d\Omega_{k'} P_{\ell}(\hat{k} \cdot \hat{k}') P_{\ell'}(\hat{r} \cdot \hat{k}') &= \tag{5.24} \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}(\hat{k} \cdot \hat{r}) \sqrt{\frac{4\pi}{2\ell+1}} \delta_{\ell, \ell'} \delta_{0, \ell'_z} \\
&= \frac{4\pi}{2\ell'+1} Y_0^{(\ell')*}(\hat{k} \cdot \hat{r}) \sqrt{\frac{4\pi}{2\ell+1}} \delta_{\ell, \ell'} = \frac{4\pi}{2\ell+1} P_{\ell}(\hat{k} \cdot \hat{r}) \delta_{\ell, \ell'} .
\end{aligned}$$

On substitution of the result (5.24) into the expression (5.20) one finds

$$\begin{aligned}
f(\vec{k}, \hat{r}) &= -4\pi^2 \mu \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) \int_0^{\infty} dk' T_{\ell}(k, k') \delta(k - k') \\
&= -4\pi^2 \mu \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) T_{\ell}(k) \quad .
\end{aligned} \tag{5.25}$$

For the relation between the transition amplitude and the partial wave phase shifts one has the following formulas (see [1] in formulas 11.59 to 11.62):

$$\begin{aligned}
f(\vec{k}, \hat{r}) &= \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) \frac{S_{\ell}(k) - 1}{2ik} \\
&= \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) \frac{e^{2i\delta_{\ell}(k)} - 1}{2i} \\
&= \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) e^{i\delta_{\ell}(k)} \sin(\delta_{\ell}(k)) \\
&= \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{r}) \frac{1}{\cotg(\delta_{\ell}(k)) - i} \quad ,
\end{aligned} \tag{5.26}$$

from which one moreover may deduce, that for a spherically symmetric local potential holds the relation

$$-4\pi^2 \mu T_{\ell}(k) = \frac{S_{\ell}(k) - 1}{2ik} \quad . \tag{5.27}$$

5.3 The delta-shell potential

Let us consider the following one-channel Schrödinger equation

$$\frac{1}{2\mu} \left\{ -\nabla^2 + \frac{\lambda}{a} \delta(r-a) \right\} \psi(\vec{r}) = E \psi(\vec{r}) \quad \text{for } a > 0 \quad . \quad (5.28)$$

Inside ($r < a$) and outside ($r > a$) the sphere of radius a the scattered particles feel no interaction. Hence, their equation of motion inside and outside the sphere is given by

$$-\frac{\nabla^2}{2\mu} \psi(\vec{r}) = E \psi(\vec{r}) \quad \text{for } r < a \quad \text{and} \quad r > a \quad , \quad (5.29)$$

which is the equation of motion for a freely moving particle.

Since the delta-shell potential is spherically symmetric, we may assume that its solutions have definite quantum numbers, ℓ and ℓ_z , for respectively angular momentum and its z component. When we define the radial wave function $u_\ell(r)$ by

$$\psi(\vec{r}) = \frac{u_\ell(r)}{r} Y_{\ell_z}^{(\ell)}(\vartheta, \varphi) \quad , \quad (5.30)$$

then we find for the radial partial wave equation the expression

$$\frac{1}{2\mu} \left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{\lambda}{a} \delta(r-a) \right] u_\ell(r) = E u_\ell(r) \quad . \quad (5.31)$$

At $r = a$ one obtains the following boundary conditions:

$$u_\ell(r \uparrow a) = u_\ell(r \downarrow a) \quad \text{and} \quad \frac{1}{2\mu} \left(-\left. \frac{d u_\ell(r)}{dr} \right|_{r \downarrow a} + \left. \frac{d u_\ell(r)}{dr} \right|_{r \uparrow a} + \frac{\lambda}{a} u_\ell(a) \right) = 0 \quad . \quad (5.32)$$

The second boundary condition of formula (5.32), which implies that the derivative of the wave function is discontinuous at $r = a$, is found by integrating wave equation (5.31) at an infinitesimal interval including the point $r = a$, *i.e.*

$$\lim_{\epsilon \downarrow 0} \int_{a-\epsilon}^{a+\epsilon} dr \left\{ \frac{1}{2\mu} \left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{\lambda}{a} \delta(r-a) \right] u_\ell(r) = E u_\ell(r) \right\} \quad ,$$

thereby noticing that in the limit $\epsilon \downarrow 0$ the integrals over $u_\ell(r)$ and $u_\ell(r)/r^2$ vanish.

The first boundary condition of formula (5.32) is obtained by integrating the second boundary condition, also at an infinitesimal interval which includes the point $r = a$.

Further boundary conditions are the usual: The radial wave function $u_\ell(r)$ vanishes at the origin ($r = 0$) and must have oscillating behavior at infinity ($r \rightarrow \infty$) since it describes a freely moving scattered particle.

The differential equation of formula (5.31) is for $\lambda = 0$ solved by spherical Bessel (J) and Neumann (N) functions, the first of which behaves well at the origin. A precise definition of those functions is given below.

Let us first recall that the differential equation

$$\frac{1}{2\mu} \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) u_\ell = E u_\ell \quad , \quad (5.33)$$

is solved by the following two linearly independent functions

$$J_\ell(kr) = k^{-\ell} r j_\ell(kr) \quad \text{and} \quad N_\ell(kr) = k^{\ell+1} r n_\ell(kr) \quad , \quad (5.34)$$

where the linear momentum k is defined by

$$k^2 = 2\mu E \quad (5.35)$$

and where j_ℓ and n_ℓ are the spherical Bessel and Neumann functions, respectively, the properties of which can be found in any textbook on Quantum Mechanics (see e.g. [1] pages 194 ff). The solution $J_\ell(kr)$ satisfies the usual boundary conditions at the origin, *i.e.* $J_\ell(r \rightarrow 0) \rightarrow 0$.

For the solutions (5.34) one has the following Wronskian relation

$$W(J_\ell(ka), N_\ell(ka)) = \left[J_\ell(r) \frac{dN_\ell(r)}{dr} - \frac{dJ_\ell(r)}{dr} N_\ell(r) \right]_{r \rightarrow a} = 1 \quad . \quad (5.36)$$

A general solution of the Schrödinger equation (5.31), which moreover satisfies the boundary conditions at the origin and at infinity, is given by

$$u_\ell(r) = \begin{cases} A J_\ell(kr) & r < a \\ B [J_\ell(kr) k^{2\ell+1} \cotg(\delta_\ell(E)) - N_\ell(kr)] & r > a \end{cases} \quad (5.37)$$

where A , and B are normalization constants, which are not independent because of the boundary conditions (5.32).

From the first boundary condition of formula (5.32) we derive the following equation

$$A J_\ell(ka) = B [J_\ell(ka) k^{2\ell+1} \cotg(\delta_\ell(E)) - N_\ell(ka)] \quad . \quad (5.38)$$

Whereas, from the second boundary condition of formula (5.32) one obtains

$$\frac{1}{2\mu} \left\{ -B [J'_\ell(ka) k^{2\ell+1} \cotg(\delta_\ell(E)) - N'_\ell(ka)] + A J'_\ell(ka) + \frac{\lambda}{a} A J_\ell(ka) \right\} = 0 \quad , \quad (5.39)$$

where we wrote J' and N' for respectively dJ/dr and dN/dr .

By elimination of the normalization constants A and B in equations (5.38) and (5.39), one obtains

$$\frac{1}{2\mu} \left\{ W(J_\ell(ka), N_\ell(ka)) + \frac{\lambda}{a} J_\ell(ka) [J_\ell(ka) k^{2\ell+1} \cotg(\delta_\ell(E)) - N_\ell(ka)] \right\} = 0 \quad .$$

Using furthermore the Wronskian relation (5.36), we arrive for the cotangent of the phase shift at

$$k^{2\ell+1} \cotg(\delta_\ell(E)) = \frac{N_\ell(ka)}{J_\ell(ka)} - \frac{a}{\lambda J_\ell^2(ka)} \quad ,$$

or, similarly, in terms of the usual spherical Bessel and Neumann functions

$$\cotg(\delta_\ell(E)) = \frac{n_\ell(ka)}{j_\ell(ka)} - \frac{1}{\lambda k a j_\ell^2(ka)} \quad . \quad (5.40)$$

The transition matrix elements of the partial wave scattering operator, S_ℓ , defined by (see e.g. [1], formula 11.67)

$$S_\ell(k) = e^{2i\delta_\ell(E(k))} \quad , \quad (5.41)$$

are then readily determined by

$$S_\ell(k) = \frac{\cotg(\delta_\ell) + i}{\cotg(\delta_\ell) - i} = \frac{1 - i\lambda k a j_\ell(ka) h_\ell^{(2)}(ka)}{1 + i\lambda k a j_\ell(ka) h_\ell^{(1)}(ka)} \quad . \quad (5.42)$$

The spherical Hankel functions, $h_\ell^{(1)}$ and $h_\ell^{(2)}$, of respectively the first and the second kind, are defined by

$$h_\ell^{(1)}(z) = j_\ell(z) + in_\ell(z) \quad \text{and} \quad h_\ell^{(2)}(z) = j_\ell(z) - in_\ell(z) \quad . \quad (5.43)$$

Notice that the limit $\lambda \rightarrow \infty$ yields the usual expressions for scattering from an infinitely hard sphere of radius $r = a$, *i.e.*

$$\cotg(\delta_\ell(E)) = \frac{n_\ell(ka)}{j_\ell(ka)} \quad \text{and} \quad S_\ell(k) = \frac{h_\ell^{(2)}(ka)}{h_\ell^{(1)}(ka)} \quad , \quad (5.44)$$

since indeed the inner region of the delta-shell becomes inaccessible for scattering when the coupling constant λ grows infinitely large.

For later use we also determine the on-shell matrix elements of the partial wave transition operator, T_ℓ , which is defined in formula (5.19). Here we obtain

$$T_\ell(k) = - \left(\frac{1}{4\pi^2 k \mu} \right) \frac{1}{\cotg(\delta_\ell) - i} = \left(\frac{1}{4\pi^2 \mu} \right) \frac{\lambda a j_\ell^2(ka)}{1 + i\lambda k a j_\ell(ka) h_\ell^{(1)}(ka)} \quad . \quad (5.45)$$

The relation of those quantities to the scattering amplitude is given in formula (5.25). Here we find

$$f(k, \Omega) = -4\pi^2 \mu \sum_{\ell=0}^{\infty} (2\ell + 1) T_\ell(k) P_\ell(\Omega) \quad . \quad (5.46)$$

For the differential cross section, defined in formula (3.24), and the total cross section we have moreover the relations

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f(k, \Omega)|^2 = (4\pi^2 \mu)^2 \left| \sum_{\ell=0}^{\infty} (2\ell + 1) T_\ell(k) P_\ell(\Omega) \right|^2 \quad , \\ \text{and} \quad \sigma &= \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi (4\pi^2 \mu)^2 \sum_{\ell=0}^{\infty} (2\ell + 1) |T_\ell(k)|^2 \quad . \end{aligned} \quad (5.47)$$

5.4 The T -operator

From the Lippmann-Schwinger equation (4.56) we deduce for the matrix elements of the T -operator the following relation

$$\langle \vec{p} | T(z) | \vec{p}' \rangle = \langle \vec{p} | V | \vec{p}' \rangle + \int d^3k \int d^3k' \langle \vec{p} | V | \vec{k} \rangle \langle \vec{k} | G_0(z) | \vec{k}' \rangle \langle \vec{k}' | T(z) | \vec{p}' \rangle , \quad (5.48)$$

or equivalently

$$T(\vec{p}, \vec{p}' ; z) = V(\vec{p}, \vec{p}') + \int d^3k \int d^3k' V(\vec{p}, \vec{k}) G_0(\vec{k}, \vec{k}' ; z) T(\vec{k}', \vec{p}' ; z) , \quad (5.49)$$

which relation can formally be solved by iteration, *i.e.*

$$\begin{aligned} T(\vec{p}, \vec{p}' ; z) &= V(\vec{p}, \vec{p}') + \\ &+ \int d^3k \int d^3k' V(\vec{p}, \vec{k}) G_0(\vec{k}, \vec{k}' ; z) V(\vec{k}', \vec{p}') + \\ &+ \int d^3k \int d^3k' \int d^3k'' \int d^3k''' V(\vec{p}, \vec{k}) G_0(\vec{k}, \vec{k}' ; z) V(\vec{k}', \vec{k}'') \times \\ &\times G_0(\vec{k}'', \vec{k}''' ; z) V(\vec{k}''', \vec{p}') + \dots . \end{aligned} \quad (5.50)$$

The Green's operator $G_0(z)$, corresponding to the self-adjoint free Hamiltonian $H_0 = k^2/2\mu$ (see formula 5.7), is defined in formula (4.23). Here we find

$$G_0(\vec{k}, \vec{k}' ; z) = \langle \vec{k} | (z - H_0)^{-1} | \vec{k}' \rangle = \frac{2\mu}{2\mu z - k^2} \langle \vec{k} | \vec{k}' \rangle . \quad (5.51)$$

By insertion of the Green's function (5.51) in expression (5.50) and moreover take out identity operations of the form

$$1 = \int d^3k |\vec{k}\rangle \langle \vec{k}| , \quad (5.52)$$

we may obtain

$$\begin{aligned} T(\vec{p}, \vec{p}' ; z) &= V(\vec{p}, \vec{p}') + \int d^3k V(\vec{p}, \vec{k}) \frac{2\mu}{2\mu z - k^2} V(\vec{k}, \vec{p}') + \\ &+ \int d^3k \int d^3k' V(\vec{p}, \vec{k}) \frac{2\mu}{2\mu z - k^2} V(\vec{k}, \vec{k}') \frac{2\mu}{2\mu z - k'^2} V(\vec{k}', \vec{p}') + \dots . \end{aligned} \quad (5.53)$$

5.4.1 The delta-shell potential in momentum space

In formula (5.28) we introduced for the transition potential in configuration space an expression which contains a radial delta-shell, i.e.

$$\frac{\lambda}{2\mu a} \delta(r - a) \quad , \quad (5.54)$$

where a represents the radius of the shell and λ the intensity of the potential.

In the language of formula (5.8) for potentials local in configuration space this translates into a potential of the form

$$V(\vec{r}, \vec{r}') = \delta^{(3)}(\vec{r} - \vec{r}') \frac{\lambda}{2\mu a} \delta(r' - a) \quad . \quad (5.55)$$

The momentum space analogon for spherically symmetric configuration space potentials is defined in formula (5.14), which, when applied to expression (5.55), gives

$$\begin{aligned} V(\vec{k}, \vec{k}') &= \frac{1}{2\pi^2} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{k}') \int_0^{\infty} r^2 dr \frac{\lambda}{2\mu a} \delta(r - a) j_{\ell}(kr) j_{\ell}(k'r) \\ &= \frac{\lambda a}{4\pi^2 \mu} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{k} \cdot \hat{k}') j_{\ell}(ka) j_{\ell}(k'a) \quad . \end{aligned} \quad (5.56)$$

5.4.2 The T -matrix elements for the delta-shell

In formula (5.56) we found the momentum space potential V for the delta-shell configuration space potential (5.54). By substituting the righthand side of that equation in formula (5.53), also using (5.13) in order to compactify the resulting expression, we may obtain the T -matrix for that case, *i.e.*

$$\begin{aligned} T(\vec{p}, \vec{p}'; z) &= \bar{\lambda} j_0(|-\vec{p} + \vec{p}'|a) + \\ &+ \bar{\lambda}^2 \int d^3k j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{p}'|a) \\ &+ \bar{\lambda}^3 \int d^3k \int d^3k' j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{k}'|a) \times \\ &\quad \times \frac{2\mu}{2\mu z - k'^2} j_0(|-\vec{k}' + \vec{p}'|a) \\ &+ \dots \quad , \end{aligned} \quad (5.57)$$

where $\bar{\lambda}$ stand for

$$\bar{\lambda} = \frac{\lambda a}{4\pi^2 \mu} \quad . \quad (5.58)$$

The Born term

The first term of the righthand side of formula (5.57) can be compared to the first term of the on-shell expression (5.45) after expanding in λ . For the latter expansion we find

$$T_\ell(p) = \frac{\lambda a j_\ell^2(pa)}{4\pi^2 \mu} \left\{ 1 - i\lambda p a j_\ell(pa) h_\ell^{(1)}(pa) + \left(i\lambda p a j_\ell(pa) h_\ell^{(1)}(pa) \right)^2 + \dots \right\} . \quad (5.59)$$

Using formula (5.13) we obtain for the first term of the righthand side of formula (5.57) the following

$$\bar{\lambda} j_0 \left(\left| -\vec{p} + \vec{p}' \right| a \right) = \frac{\lambda a}{4\pi^2 \mu} \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) j_\ell(p'a) . \quad (5.60)$$

Hence, for the Born term of T_ℓ we find

$$T_\ell^{(1)}(p, p') = \frac{\lambda a}{4\pi^2 \mu} j_\ell(pa) j_\ell(p'a) . \quad (5.61)$$

On-shell, *i.e.* $p' = p$, expression (5.61) is equal to the first term of (5.59).

The second order term

In order to perform the integration of the second term of the righthand side of formula (5.57), we start by introducing the expansion (5.13), to obtain

$$\begin{aligned} & \int d^3k j_0 \left(\left| -\vec{p} + \vec{k} \right| a \right) \frac{2\mu}{2\mu z - k^2} j_0 \left(\left| -\vec{k} + \vec{p}' \right| a \right) = \quad (5.62) \\ & = \sum_{\ell, \ell'=0}^{\infty} (2\ell + 1)(2\ell' + 1) j_\ell(pa) j_{\ell'}(p'a) \times \\ & \quad \times 2\mu \int d^3k P_\ell(\hat{p} \cdot \hat{k}) P_{\ell'}(\hat{k} \cdot \hat{p}') \frac{j_\ell(ka) j_{\ell'}(ka)}{2\mu z - k^2} . \end{aligned}$$

The details of the \vec{k} integration are studied in subsection (5.4.3). Using the definition (5.81), we may write here

$$\begin{aligned} & \int d^3k j_0 \left(\left| -\vec{p} + \vec{k} \right| a \right) \frac{2\mu}{2\mu z - k^2} j_0 \left(\left| -\vec{k} + \vec{p}' \right| a \right) = \quad (5.63) \\ & = \sum_{\ell, \ell'=0}^{\infty} (2\ell + 1)(2\ell' + 1) j_\ell(pa) j_{\ell'}(p'a) \mathcal{I}_\ell(\vec{p}, \vec{p}'; \mu; 1) , \end{aligned}$$

which, by substitution of the result (5.88), gives

$$\int d^3k j_0 \left(\left| -\vec{p} + \vec{k} \right| a \right) \frac{2\mu}{2\mu z - k^2} j_0 \left(\left| -\vec{k} + \vec{p}' \right| a \right) = \quad (5.64)$$

$$\begin{aligned}
&= \sum_{\ell, \ell'=0}^{\infty} (2\ell+1)(2\ell'+1) j_{\ell}(pa) j_{\ell'}(p'a) \times \\
&\quad \times \left[-i \frac{4\pi^2 \mu p}{2\ell+1} \delta_{\ell, \ell'} P_{\ell}(\hat{p} \cdot \hat{p}') j_{\ell}(pa) h_{\ell}^{(1)}(pa) \right] , \tag{5.65}
\end{aligned}$$

Putting everything together amounts for the second term on the righthand side of formula (5.57) to

$$\begin{aligned}
&\bar{\lambda}^2 \int d^3k j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{p}'|a) = \\
&= -\frac{i\lambda^2 p a^2}{4\pi^2 \mu} \sum_{\ell=0}^{\infty} (2\ell+1) j_{\ell}^2(pa) h_{\ell}^{(1)}(pa) j_{\ell}(p'a) P_{\ell}(\hat{p} \cdot \hat{p}') , \tag{5.66}
\end{aligned}$$

or equivalently, for the second order in λ term of T_{ℓ} ,

$$T_{\ell}^{(2)}(p, p') = -\frac{i\lambda^2 p a^2}{4\pi^2 \mu} j_{\ell}^2(pa) h_{\ell}^{(1)}(pa) j_{\ell}(p'a) . \tag{5.67}$$

This term may be compared to the second term of the on-shell expansion (5.59). We find again perfect agreement.

The third order term

For the integrations of the third term of the righthand side of formula (5.57), we may, of course, use the results of section (5.4.2). We start then with the \vec{k} -integration, *i.e.*

$$\int d^3k j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{k}'|a) , \tag{5.68}$$

for which we recognize the expression (5.62) after the substitution p' by k' . Accordingly, using formula (5.67), we write

$$\begin{aligned}
&\int d^3k j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{k}'|a) = \\
&= -4i\pi^2 p \mu \sum_{\ell=0}^{\infty} (2\ell+1) j_{\ell}^2(pa) h_{\ell}^{(1)}(pa) j_{\ell}(k'a) P_{\ell}(\hat{p} \cdot \hat{k}') . \tag{5.69}
\end{aligned}$$

Hence, we obtain for the third term of the righthand side of formula (5.57) the following

$$\begin{aligned}
&\int d^3k \int d^3k' j_0(|-\vec{p} + \vec{k}|a) \frac{2\mu}{2\mu z - k^2} j_0(|-\vec{k} + \vec{k}'|a) \frac{2\mu}{2\mu z - k'^2} j_0(|-\vec{k}' + \vec{p}'|a) \\
&= -4i\pi^2 p \mu \sum_{\ell=0}^{\infty} (2\ell+1) j_{\ell}^2(pa) h_{\ell}^{(1)}(pa) \int d^3k' j_{\ell}(k'a) P_{\ell}(\hat{p} \cdot \hat{k}') \frac{2\mu}{2\mu z - k'^2} j_0(|-\vec{k}' + \vec{p}'|a) \tag{5.70}
\end{aligned}$$

Here we introduce once more expansion (5.13) and moreover definition (5.81), to obtain for the integration piece of formula (5.70), the result

$$\begin{aligned}
& \int d^3 k' j_\ell(k'a) P_\ell(\hat{p} \cdot \hat{k}') \frac{2\mu}{2\mu z - k'^2} j_0\left(\left|-\vec{k}' + \vec{p}'\right|a\right) = \\
& = \int d^3 k' j_\ell(k'a) P_\ell(\hat{p} \cdot \hat{k}') \frac{2\mu}{2\mu z - k'^2} \sum_{\ell'=0}^{\infty} (2\ell' + 1) P_{\ell'}(\hat{k}' \cdot \hat{p}') j_{\ell'}(k'a) j_{\ell'}(p'a) \\
& = \sum_{\ell'=0}^{\infty} (2\ell' + 1) j_{\ell'}(p'a) \mathcal{I}_\ell(\vec{p}, \vec{p}'; \mu; 1) .
\end{aligned} \tag{5.71}$$

The final integration is given in formula (5.88). So, we find for the third term of the righthand side of formula (5.57) the following expression

$$\begin{aligned}
& \bar{\lambda}^3 \int d^3 k \int d^3 k' j_0\left(\left|-\vec{p} + \vec{k}\right|a\right) \frac{2\mu}{2\mu z - k^2} j_0\left(\left|-\vec{k} + \vec{k}'\right|a\right) \frac{2\mu}{2\mu z - k'^2} j_0\left(\left|-\vec{k}' + \vec{p}'\right|a\right) \\
& = -\frac{\lambda^3 p^2 a^3}{4\pi^2 \mu} \sum_{\ell=0}^{\infty} (2\ell + 1) j_\ell^3(pa) h_\ell^{(1)2}(pa) j_\ell(p'a) P_\ell(\hat{p} \cdot \hat{p}') .
\end{aligned} \tag{5.72}$$

or equivalently, for the third order in λ term of T_ℓ ,

$$T_\ell^{(3)}(p, p') = -\frac{\lambda^3 p^2 a^3}{4\pi^2 \mu} j_\ell^3(pa) h_\ell^{(1)2}(pa) j_\ell(p'a) . \tag{5.73}$$

This term may be compared to the third term of the on-shell expansion (5.59). We find once more perfect agreement.

The $n + 1$ -th order term

By comparing the previous results given in formulas (5.60), (5.66) and (5.72), we may expect for the $(n + 1)$ -th term of expansion (5.57) the following expression

$$\begin{aligned}
& T^{(n+1)}(\vec{p}, \vec{p}') = \\
& = \bar{\lambda} (-i\lambda pa)^n \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) j_\ell(p'a) \left[j_\ell(pa) h_\ell^{(1)}(pa) \right]^n ,
\end{aligned} \tag{5.74}$$

where $\bar{\lambda}$ is as defined in formula (5.58).

This can easily be verified as we will show below. From expansion (5.57) we observe for the relation of two subsequent terms the following identity

$$T^{(n+1)}(\vec{p}, \vec{p}') = \bar{\lambda} \int d^3 k T^{(n)}(\vec{p}, \vec{k}) \frac{2\mu}{2\mu z - k^2} j_0\left(\left|-\vec{k} + \vec{p}'\right|a\right) . \tag{5.75}$$

When we substitute here expression (5.74) and formula (5.13), also using definition (5.58), then we find

$$\begin{aligned}
T^{(n+1)}(\vec{p}, \vec{p}') &= \bar{\lambda} \int d^3k \bar{\lambda} (-i\lambda pa)^{n-1} \times \\
&\times \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{k}) j_{\ell}(pa) j_{\ell}(ka) [j_{\ell}(pa) h_{\ell}^{(1)}(pa)]^{n-1} \times \\
&\times \frac{2\mu}{2\mu z - k^2} \sum_{\ell'=0}^{\infty} (2\ell' + 1) P_{\ell'}(\hat{k} \cdot \hat{p}') j_{\ell'}(ka) j_{\ell'}(p'a) . \quad (5.76)
\end{aligned}$$

Using furthermore the result (5.88), we obtain

$$\begin{aligned}
T^{(n+1)}(\vec{p}, \vec{p}') &= \bar{\lambda}^2 (-i\lambda pa)^{n-1} (-i4\pi^2\mu p) \times \\
&\times \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') j_{\ell}(pa) j_{\ell}(p'a) [j_{\ell}(pa) h_{\ell}^{(1)}(pa)]^{n-1} j_{\ell}(pa) h_{\ell}^{(1)}(pa) , \quad (5.77)
\end{aligned}$$

which, by substitution of the definition (5.58), gives indeed expression (5.74).

The full matrix elements

From the above results one can read off the expression for the full sum of all terms of formula (5.57) for the matrix elements of the T -operator, *i.e.*

$$\begin{aligned}
T(\vec{p}, \vec{p}') &= \sum_{n=1}^{\infty} T^{(n)}(\vec{p}, \vec{p}') \quad (5.78) \\
&= \bar{\lambda} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') j_{\ell}(pa) j_{\ell}(p'a) \sum_{n=0}^{\infty} (-i\lambda pa)^n [j_{\ell}(pa) h_{\ell}^{(1)}(pa)]^n \\
&= \frac{\lambda a}{4\pi^2\mu} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') \frac{j_{\ell}(pa) j_{\ell}(p'a)}{1 + i\lambda pa j_{\ell}(pa) h_{\ell}^{(1)}(pa)} .
\end{aligned}$$

Notice that the above expression (5.78) is indeed of the form (5.19). We may thus arrive at the scattering amplitude by substitution of the on-shell (*i.e.* $p' = p$) matrix elements in formula (5.25), which gives

$$f(\vec{p}, \hat{r}) = -\lambda a \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{r}) \frac{j_{\ell}^2(pa)}{1 + i\lambda pa j_{\ell}(pa) h_{\ell}^{(1)}(pa)} . \quad (5.79)$$

It is also interesting to notice that this way we may obtain an expression for the T -matrix elements of the infinitely hard sphere, by taking the limit $\lambda \rightarrow \infty$ in formula (5.78), *i.e.*

$$T(\vec{p}, \vec{p}') = -\frac{i}{4\pi^2\mu p} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') \frac{j_{\ell}(p'a)}{h_{\ell}^{(1)}(pa)} . \quad (5.80)$$

A direct calculation of those matrix elements might be impossible, since expression (5.14) becomes infinite in the limit of $V(r) \rightarrow \infty$ for $r < a$.

5.4.3 Details of the \vec{k} integration

Let us study the following integration

$$\begin{aligned}
\mathcal{I}_\ell(\vec{p}, \vec{p}'; \mu; f_\ell) &= \tag{5.81} \\
&= 2\mu \int d^3k' P_\ell(\hat{p} \cdot \hat{k}) P_{\ell'}(\hat{k} \cdot \hat{p}') \frac{j_\ell(ka) j_{\ell'}(ka)}{2\mu z - k^2} f_\ell(k^2) \\
&= 2\mu \int d\Omega_k P_\ell(\hat{p} \cdot \hat{k}) P_{\ell'}(\hat{k} \cdot \hat{p}') \int_0^\infty k^2 dk \frac{j_\ell(ka) j_{\ell'}(ka)}{2\mu z - k^2} f_\ell(k^2) \quad ,
\end{aligned}$$

where f_ℓ represents an arbitrary well-behaved function of linear momentum squared.

For the integration over the angles we may use formula (5.24), *i.e.*

$$\int d\Omega_k P_\ell(\hat{p} \cdot \hat{k}) P_{\ell'}(\hat{k} \cdot \hat{p}') = \frac{4\pi}{2\ell + 1} P_\ell(\hat{p} \cdot \hat{p}') \delta_{\ell, \ell'} \quad . \tag{5.82}$$

Next, we must concentrate on the radial integration, *i.e.*

$$\int_0^\infty k^2 dk \frac{j_\ell^2(ka)}{2\mu z - k^2} f_\ell(k^2) \quad . \tag{5.83}$$

Integrals of this type appear (for example at page 46 of the Ph.D. thesis of George Rupp [3]) in perturbative calculus for the meson-meson scattering model which we will discuss next. The trick amounts to the following identity

$$\int_0^\infty k^2 dk \frac{j_\ell^2(ka)}{2\mu z - k^2} f_\ell(k^2) = \frac{1}{2} \int_{-\infty}^\infty k^2 dk \frac{j_\ell(ka) h_\ell^{(1)}(ka)}{2\mu z - k^2} f_\ell(k^2) \quad , \tag{5.84}$$

by using the following properties for the spherical Bessel and Hankel functions (the Hankel functions are defined in formula 5.43)

$$j_\ell(e^{\pi i} ka) = e^{\pi i \ell} j_\ell(ka) \quad \text{and} \quad h_\ell^{(1)}(e^{\pi i} ka) = e^{-\pi i \ell} h_\ell^{(2)}(ka) \quad . \tag{5.85}$$

For large imaginary part of the argument ka the function $h_\ell^{(1)}(ka)$ tends to zero. Therefore one can close a complex contour by joining to the real k -axis a semicircle in the complex upper half plane and determine the integration for the closed contour in the complex k -plane. The part of the semicircle does not contribute.

Finally, we define

$$2\mu z = (p + i\epsilon)^2 \quad , \tag{5.86}$$

and take the limit $\epsilon \rightarrow 0$ after integration. The integral (5.84) turns into a contour integral for which we may apply Cauchy's residue theorem as follows

$$\int_0^\infty k^2 dk \frac{j_\ell^2(ka)}{2\mu z - k^2} f_\ell(k^2) =$$

$$\begin{aligned}
&= \lim_{\epsilon \downarrow 0} \frac{1}{2} \int_{-\infty}^{\infty} k^2 dk \frac{j_\ell(ka) h_\ell^{(1)}(ka)}{(p+i\epsilon-k)(p+i\epsilon+k)} f_\ell(k^2) \\
&= \frac{1}{2} 2\pi i \frac{-p^2}{2p} j_\ell(pa) h_\ell^{(1)}(pa) f_\ell(p^2) = -\frac{i\pi p}{2} j_\ell(pa) h_\ell^{(1)}(pa) f_\ell(p^2) \quad , \quad (5.87)
\end{aligned}$$

Putting everything together, we find for the integration of formula (5.81) the following result

$$\mathcal{I}_\ell(\vec{p}, \vec{p}' ; \mu ; f_\ell) = -i \frac{4\pi^2 \mu p}{2\ell + 1} \delta_{\ell, \ell'} P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) h_\ell^{(1)}(pa) f_\ell(p^2) \quad . \quad (5.88)$$

5.5 Meson-meson scattering

For a second example we study a model for the scattering of interacting composite particles (see for example [4]).

5.5.1 Introduction

Imagine in the far past a pair of composite particles heading towards the interaction region, which, evidently, is also the centre of mass of this system. In the far future we imagine a number of such objects flying away from the interaction region.

For the structure of our composite particles, which we will refer to as *mesons* in the following, we have the following picture: Their elementary constituents we will call *valence quarks*, denoted by q , and *valence antiquarks*, denoted by \bar{q} . In this report we do not consider different flavors, neither color, nor spin. Each meson consists of one valence quark and one valence antiquark confined by a harmonic oscillator force. Equivalently, one may represent a meson by a spring which at one endpoint is connected to a valence quark and at the other endpoint to a valence antiquark.

Mesons are here assumed to interact by the phenomenon of quark pair creation, which is the process in which one valence quark and one valence antiquark are created from the vacuum. In that case the spring breaks up in order to form two mesons. In the opposite process, where one valence quark of one meson annihilates with one valence antiquark of the other meson, two springs fuse in order to form one meson. Other processes will not be considered here.

Moreover, here we will restrict ourselves to final states with two mesons, *i.e.*

$$A + B \longrightarrow C + D \quad . \quad (5.89)$$

Consequently, we assume that in the interaction region two mesons may fuse to one meson, or break up into two mesons. But, due to the restriction (5.89) one has always at most two and minimally one meson in the interaction region. The latter situation can only exist around the origin, which represents the centre of mass of the system. We will describe this by the one-particle harmonic oscillator, which is equivalent to the relative motion of one valence quark and one valence antiquark confined by a spring.

For the two-meson situation we assume that the quantum numbers are the only relevant parameters of each of the two mesons, which hence can then be described by point particles.

The only interactions we allow for, are spring fusion when there are two mesons in the interaction region, and spring fission into two mesons when there is one meson in the interaction region. The probability of those processes to occur will be given by the distributions of the end points of the springs, or, equivalently, by the quark and the antiquark distributions.

The wave function for such a system must describe the probability that we find the system in the one-meson state, as well as the probability that we find the system in the two-meson state. This can conveniently be done by defining a two-component wave function, given by

$$\begin{pmatrix} \psi_c \\ \psi_f \end{pmatrix} , \quad (5.90)$$

where $|\psi_c|^2$ represents the probability to find the system in the one-meson state and $|\psi_f|^2$ the probability to find the system in the two-meson state. Evidently, because of the above described assumptions and, in particular, because of assumption (5.89), the two components of (5.90) must satisfy here the following condition:

$$|\psi_c|^2 + |\psi_f|^2 = 1 \quad . \quad (5.91)$$

5.5.2 The wave equation for the model

We assume that the system (5.90) can be described by a stationary 2×2 non-relativistic wave equation of the following form (in units $c = 1$)

$$\begin{pmatrix} H_c & U(\vec{r}) \\ U(\vec{r}) & H_f \end{pmatrix} \begin{pmatrix} \psi_c(\vec{r}) \\ \psi_f(\vec{r}) \end{pmatrix} = E \begin{pmatrix} \psi_c(\vec{r}) \\ \psi_f(\vec{r}) \end{pmatrix} \quad . \quad (5.92)$$

The dynamics of the one-meson state is contained in H_c , whereas H_f describes the dynamics of the two-meson state. The potential U describes the transitions from one mode of the model to the other mode.

In the absence of spring fission or fusion processes, the transition potential U vanishes. In that case the two channels decouple and the system is either described by a stationary meson at the origin, or by a system of two non-interacting mesons. Hence, since the one-meson state is assumed to be described by a valence pair of quark and antiquark confined by a harmonic oscillator force, H_c must be of the following form:

$$H_c = -\frac{\nabla^2}{2\mu_c} + m_q + m_{\bar{q}} + \frac{1}{2}\mu_c\omega^2 r^2 \quad , \quad (5.93)$$

where m_q and $m_{\bar{q}}$ represent the masses of respectively the quark and the antiquark, where ω represents the oscillator frequency and where μ_c stands for the reduced mass of the quark+antiquark system. Moreover, since the two-meson state describes a system of two non-interacting mesons, H_f is just the free particle Hamiltonian, according to the relation

$$H_f = -\frac{\nabla^2}{2\mu_f} + M_1 + M_2 \quad , \quad (5.94)$$

where M_1 and M_2 represent the meson masses and μ_f the reduced mass of the two-meson system.

Interaction is achieved by considering a non-zero transition potential U . We will assume that such potential vanishes at the origin and at large distances and has some maximum at an intermediate distance which is of the order of the size of a meson. A transition potential U which has such characteristics can conveniently be approximated by a delta-shell, *i.e.*

$$U(\vec{r}) = \lambda V(r) \quad \text{where} \quad V(r) = \frac{1}{2\mu_c a} \delta(r - a) \quad . \quad (5.95)$$

Here we will study the behavior of the solutions of wave equation (5.92) in the approximation (5.95) for the transition potential.

5.5.3 The radial wave equation

The 2×2 Hamiltonian operator of equation (5.92) is rotational invariant, as can be concluded from the expressions (5.93), (5.94) and (5.95). Consequently, it is useful to introduce angular momentum, \vec{L} , and write

$$\begin{pmatrix} \psi_c(\vec{r}) \\ \psi_f(\vec{r}) \end{pmatrix} = \begin{pmatrix} \frac{u_c(r)}{r} Y_{\ell_z}^{(\ell)}(\vartheta, \varphi) \\ \frac{u_f(r)}{r} Y_{\ell_z}^{(\ell)}(\vartheta, \varphi) \end{pmatrix} . \quad (5.96)$$

Substitution of equation (5.96) into the wave equation (5.92), also using the relations (5.93), (5.94) and (5.95), leads to the following system of coupled differential equations for the radial parts of wave function

$$\begin{pmatrix} h_c & \lambda V(r) \\ \lambda V(r) & h_f \end{pmatrix} \begin{pmatrix} u_c \\ u_f \end{pmatrix} = E \begin{pmatrix} u_c \\ u_f \end{pmatrix} , \quad (5.97)$$

where

$$h_c = \frac{1}{2\mu_c} \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) + m_q + m_{\bar{q}} + \frac{1}{2}\mu_c\omega^2 r^2 ,$$

$$h_f = \frac{1}{2\mu_f} \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) + M_1 + M_2$$

and

$$V = \frac{1}{2\mu_c a} \delta(r - a) . \quad (5.98)$$

5.5.4 Coupled channel wave equation with one delta shell

In this section we study the solutions of the 2×2 radial wave equation with one delta shell which is defined in formula (5.98). For $r < a$ and for $r > a$ one has to solve the two uncoupled differential equations, equivalent to $\lambda = 0$, given by

$$\begin{pmatrix} h_c & 0 \\ 0 & h_f \end{pmatrix} \begin{pmatrix} u_c \\ u_f \end{pmatrix} = E \begin{pmatrix} u_c \\ u_f \end{pmatrix} . \quad (5.99)$$

At $r = a$ one may obtain the following boundary conditions:

$$\begin{cases} \frac{1}{2\mu_c} \left(-\frac{d u_c(r)}{dr} \Big|_{r \downarrow a} + \frac{d u_c(r)}{dr} \Big|_{r \uparrow a} \right) + \frac{\lambda}{2\mu_c a} u_f(a) = 0 \\ \frac{\lambda}{2\mu_c a} u_c(a) + \frac{1}{2\mu_f} \left(-\frac{d u_f(r)}{dr} \Big|_{r \downarrow a} + \frac{d u_f(r)}{dr} \Big|_{r \uparrow a} \right) = 0 \end{cases} , \quad (5.100)$$

by integrating wave equation (5.98) at an infinitesimal interval including the point $r = a$, *i.e.*

$$\lim_{\epsilon \downarrow 0} \int_{a-\epsilon}^{a+\epsilon} dr \left\{ \begin{pmatrix} h_c & \lambda V \\ \lambda V & h_f \end{pmatrix} \begin{pmatrix} u_c \\ u_f \end{pmatrix} = E \begin{pmatrix} u_c \\ u_f \end{pmatrix} \right\} ,$$

and

$$\begin{cases} u_c(r \uparrow a) = u_c(r \downarrow a) \\ u_f(r \uparrow a) = u_f(r \downarrow a) \end{cases} , \quad (5.101)$$

by integrating equation (5.100) also at an infinitesimal interval which includes the point $r = a$.

Further boundary conditions are the usual: The wave functions u_c and u_f both vanish at the origin. At infinity the wave function u_c must be damped exponentially, since u_c describes a confined system, whereas, above threshold ($E > M_1 + M_2$), the wave function u_f must have oscillating behavior, since u_f describes the scattered mesons.

Let us denote by F_c and G_c the solutions of the upper differential equation of formula (5.99) which respectively vanish at the origin and damp exponentially at infinity. Below we give a precise definition of those functions.

Let us first recall that the differential equation

$$\left[\frac{1}{2\mu} \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) + m_1 + m_2 + \frac{1}{2}\mu\omega^2 r^2 \right] u = E u , \quad (5.102)$$

is solved by the following two linearly independent functions

$$F(r) = \frac{1}{\Gamma\left(\ell + \frac{3}{2}\right)} (\mu\omega r^2)^{(\ell+1)/2} e^{-\frac{1}{2}\mu\omega r^2} \phi\left(-\nu; \ell + \frac{3}{2}; \mu\omega r^2\right)$$

and (5.103)

$$G(r) = -\frac{1}{2}\Gamma(-\nu) r (\mu\omega r^2)^{\ell/2} e^{-\frac{1}{2}\mu\omega r^2} \psi\left(-\nu; \ell + \frac{3}{2}; \mu\omega r^2\right) ,$$

where the radial quantum number ν is defined by the following relation

$$E = \omega \left(2\nu + \ell + \frac{3}{2} \right) + m_1 + m_2 \quad , \quad (5.104)$$

and where the functions ϕ and ψ are defined by (see [5] pages 248 and 257)

$$\phi(a; b; z) = \sum_{n=0}^{\infty} \frac{(a)_n z^n}{(b)_n n!} \quad \text{with} \quad (a)_0 = 1 \quad \text{and} \quad (a)_{n+1} = (a+n)(a)_n$$

and

$$(5.105)$$

$$\psi(a; b; z) = \frac{\Gamma(1-b)}{\Gamma(a-b+1)} \phi(a; b; z) + \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b} \phi(a-b+1; 2-b; z) \quad .$$

The solution $F(r)$ is regular at the origin, but is irregular at infinity, except for some special cases known as the harmonic oscillator spectrum, whereas $G(r)$ behaves regular at infinity but not in the origin.

For the solutions (5.103) one has the following Wronskian relation

$$W(F_c(a), G_c(a)) = \left[F_c(r) \frac{d G_c(r)}{dr} - \frac{d F_c(r)}{dr} G_c(r) \right]_{r \rightarrow a} = 1 \quad (5.106)$$

The lower differential equation of formula (5.99) is solved by spherical Bessel (J) and Neumann (N) functions, discussed in formulas (5.34ff).

A general solution of the Schrödinger equation (5.98), which moreover satisfies the boundary conditions at the origin and at infinity, is given by

$$\begin{pmatrix} u_c(r) \\ u_f(r) \end{pmatrix} = \begin{cases} \begin{pmatrix} F_c(r) A_c \\ J_\ell(kr) A_f \end{pmatrix} & r < a \\ \begin{pmatrix} G_c(r) B_c \\ [J_\ell(kr) k^{2\ell+1} \cotg(\delta_\ell(E)) - N_\ell(kr)] B_f \end{pmatrix} & r > a \end{cases} \quad (5.107)$$

where A_c, A_f, B_c and B_f are normalization constants, which are not independent because of the boundary conditions (5.100) and (5.101) and where k is defined by

$$k^2 = 2\mu_f (E - M_1 - M_2) \quad . \quad (5.108)$$

From the boundary conditions (5.101) we derive the following equations

$$\begin{aligned} F_c(a) A_c &= G_c(a) B_c \quad , \\ J_\ell(ka) A_f &= [J_\ell(ka) k^{2\ell+1} \cotg(\delta_\ell(E)) - N_\ell(ka)] B_f \quad . \end{aligned} \quad (5.109)$$

Whereas, from boundary conditions (5.100) one obtains

$$\begin{aligned} \frac{1}{2\mu_c} (G'_c(a)B_c - F'_c(a)A_c) &= \frac{\lambda}{2\mu_c a} J_\ell(ka) A_f \quad , \\ \frac{1}{2\mu_f} \left([J'_\ell(ka) k^{2\ell+1} \cotg(\delta_\ell(E)) - N'_\ell(ka)] B_f - J'_\ell(ka) A_f \right) &= \frac{\lambda}{2\mu_c a} F_c(a) A_c \quad . \end{aligned} \quad (5.110)$$

When we multiply the first (respectively second) line of equation (5.110) by $F_c(a)$ (respectively $J_\ell(ka)$) and then substitute according to the relation in the first (respectively second) line of equation (5.109), then we obtain

$$\begin{aligned} \frac{B_c}{2\mu_c} W(F_c(a), G_c(a)) &= \frac{\lambda}{2\mu_c a} J_\ell(ka) F_c(a) A_f \quad , \\ -\frac{B_f}{2\mu_f} W(J_\ell(ka), N_\ell(ka)) &= \frac{\lambda}{2\mu_c a} J_\ell(ka) F_c(a) A_c \quad . \end{aligned}$$

Using furthermore the Wronskian relations (5.36) and (5.106), we find

$$\frac{B_c}{2\mu_c} = \frac{\lambda}{2\mu_c a} J_\ell(ka) F_c(a) A_f \quad \text{and} \quad -\frac{B_f}{2\mu_f} = \frac{\lambda}{2\mu_c a} J_\ell(ka) F_c(a) A_c \quad . \quad (5.111)$$

The relations (5.111) can be substituted into equations (5.109), after which follows easily for the cotangent of the phase shift the expression:

$$k^{2\ell+1} \cotg(\delta_\ell(E)) = \frac{N_\ell(ka)}{J_\ell(ka)} + \left[-\lambda^2 \frac{\mu_f}{\mu_c} \frac{1}{a^2} J_\ell^2(ka) F_c(a) G_c(a) \right]^{-1} \quad . \quad (5.112)$$

Using moreover the relations (5.34) and (5.103) for the various functions which are introduced in solution (5.107) and substitute furthermore the function \mathcal{A} defined by

$$\mathcal{A}(\nu, \ell; z) = z^{\ell + \frac{1}{2}} e^{-z} \frac{\phi\left(-\nu, \ell + \frac{3}{2}; z\right) \psi\left(-\nu, \ell + \frac{3}{2}; z\right)}{\Gamma\left(\ell + \frac{3}{2}\right)} \quad , \quad (5.113)$$

we arrive at

$$\cotg(\delta_\ell(E)) = \frac{n_\ell(ka)}{j_\ell(ka)} + \left[\frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} ka j_\ell^2(ka) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) \right]^{-1} \quad . \quad (5.114)$$

The scattering matrix follows by

$$\begin{aligned} \mathcal{S}_\ell(E) &= e^{2i\delta_\ell(E)} = \frac{\cotg(\delta_\ell(E)) + i}{\cotg(\delta_\ell(E)) - i} \quad (5.115) \\ &= \frac{1 + \frac{1}{2} i \lambda^2 \frac{\mu_f}{\mu_c} \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) ka j_\ell(ka) h_\ell^{(2)}(ka)}{1 - \frac{1}{2} i \lambda^2 \frac{\mu_f}{\mu_c} \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) ka j_\ell(ka) h_\ell^{(1)}(ka)} \quad , \end{aligned}$$

where the spherical Hankel functions of the first and the second kind are defined in formula (5.43).

5.5.5 Bound states and resonances

Bound states and resonances, which are described by singularities in the scattering matrix (5.115), can be computed from the condition

$$\cotg(\delta_\ell(E)) = i \quad , \quad (5.116)$$

which in this case reads

$$\frac{1}{2}i\lambda^2 \frac{\mu_f}{\mu_c} \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) k a j_\ell(ka) h_\ell^{(1)}(ka) = 1 \quad . \quad (5.117)$$

Approximate bound states and resonance positions

For small values of λ^2 the solutions of equation (5.117) can be found approximately. The reason is that then the bound states and resonances are close to the harmonic oscillator eigenstates. Hence, the values of the radial quantum number, ν , are almost non-negative integers, ν_0 . We write

$$\nu = \nu_0 + \Delta\nu \quad . \quad (5.118)$$

Now since \mathcal{A} and the spherical Bessel function in (5.117) are slowly varying functions of the energy, E , or, equivalently, the radial quantum number ν , the only rapid varying candidate that is left, is

$$\Gamma(-\nu) \approx \frac{(-1)^{\nu_0+1}}{(\nu_0)! \Delta\nu} \quad . \quad (5.119)$$

When we moreover substitute the following real and positive quantity

$$\begin{aligned} \mathcal{B}(\nu_0, \ell; \mu_c \omega a^2) &= \frac{(-1)^{\nu_0} \mu_f}{(\nu_0)! \mu_c} \mathcal{A}(\nu_0, \ell; \mu_c \omega a^2) \\ &= \frac{\mu_f}{\mu_c} (\mu_c \omega a^2)^\ell + \frac{1}{2} e^{-\mu_c \omega a^2} \frac{\Gamma(\ell + \nu_0 + \frac{3}{2})}{(\nu_0)!} \left[\frac{\phi(-\nu_0, \ell + \frac{3}{2}; \mu_c \omega a^2)}{\Gamma(\ell + \frac{3}{2})} \right]^2 , \end{aligned} \quad (5.120)$$

we arrive for the shift in the resonance energy at

$$\Delta E = 2\omega \Delta\nu \approx -i\lambda^2 \omega \mathcal{B}(\nu_0, \ell; \mu_c \omega a^2) k_0 a j_\ell(k_0 a) h_\ell^{(1)}(k_0 a) \quad , \quad (5.121)$$

where, following formulas (5.104) and (5.108), k_0 is defined by

$$k_0^2 = 2\mu_f \left[\omega \left(2\nu_0 + \ell + \frac{3}{2} \right) + m_q + m_{\bar{q}} - M_1 - M_2 \right] \quad . \quad (5.122)$$

For further studies we may distinguish two different cases:

- (1) $E_0 > M_1 + M_2$, and
- (2) $E_0 < M_1 + M_2$.

(1) **Above threshold**

When the nearby harmonic oscillator state has energy, E_0 , which exceeds the threshold energy, $M_1 + M_2$ (*i.e.* the sum of the rest masses of the scattered particles), then expression (5.121) has a **negative** imaginary part and a real part, according to

$$\Delta E \approx \lambda^2 \omega \mathcal{B}(\nu_0, \ell; \mu_c \omega a^2) k_0 a \left\{ -i j_\ell^2(k_0 a) + j_\ell(k_0 a) n_\ell(k_0 a) \right\} . \quad (5.123)$$

The resonance singularity of the scattering matrix which corresponds to this situation is depicted in figure (5.1).

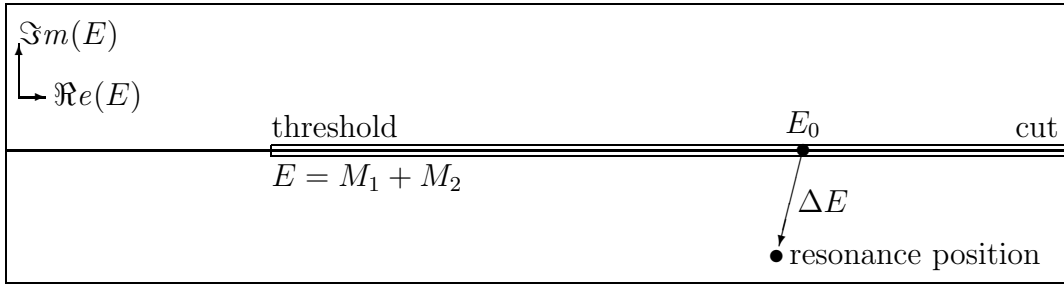


Figure 5.1: The position of a resonance singularity in the complex energy plane with respect to the harmonic oscillator state at the real energy axis.

Notice that the resonance singularity is in the lower half complex energy plane (second Riemann sheet) as it should be.

(2) Below threshold

When the nearby harmonic oscillator state has energy, E_0 , lower than the threshold energy, then expression (5.121) has only a real part. The reason is, that in that case $(k_0)^2$ is negative and hence k_0 imaginary, *i.e.*

$$k_0 = i\kappa_0 \quad (\kappa_0 \text{ real}) \quad . \quad (5.124)$$

Moreover, $\kappa_0 > 0$, because, since it describes a system of bounded scattering particles, the wavefunction ψ_f of the scattering channel must be damped exponentially, not explode.

Now in formula (48) of section 7.2.7 from [5], we find the following expansion:

$$\begin{aligned} izj_\ell(z)h_\ell^{(1)}(z) &= \frac{\pi}{2} \left\{ \frac{i}{2} z \left(\frac{1}{4}z^2\right)^\ell \sum_m \frac{\left(-\frac{1}{4}z^2\right)^m \Gamma(2\ell + 2m + 2)}{m! \left[\Gamma\left(\ell + m + \frac{3}{2}\right)\right]^2 \Gamma(2\ell + m + 2)} + \right. \\ &\quad \left. + (-1)^\ell \sum_m \frac{\left(-\frac{1}{4}z^2\right)^m \Gamma(2m + 1)}{[m!]^2 \Gamma\left(\ell + m + \frac{3}{2}\right) \Gamma\left(-\ell + m + \frac{1}{2}\right)} \right\} , \quad (5.125) \end{aligned}$$

which for $z = i\kappa_0 a$ is obviously real.

The bound state singularity of the scattering matrix which corresponds to this situation is depicted in figure (5.2).

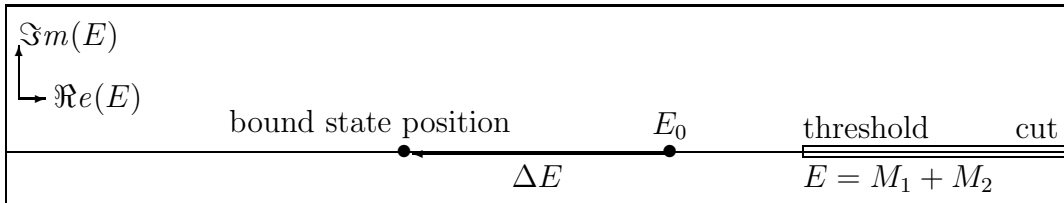


Figure 5.2: The position of a bound state singularity in the complex energy plane with respect to the harmonic oscillator state at the real energy axis.

Notice that the bound state singularity is at the real axis of the complex energy plane, as it should be.

5.6 The T -matrix for the meson-meson model

In configuration space we may write the non-relativistic 2×2 stationary matrix wave equation (5.92), also using relations (5.93), (5.94) and (5.95), in the following form

$$\begin{aligned} \left(-\frac{\nabla_r^2}{2\mu_c} + m_q + m_{\bar{q}} + \frac{1}{2}\mu_c\omega^2 r^2 - E \right) \psi_c(\vec{r}) &= -\frac{\lambda}{2\mu_c a} \delta(r-a) \psi_f(\vec{r}) \quad , \\ \left(-\frac{\nabla_r^2}{2\mu_f} + M_1 + M_2 - E \right) \psi_f(\vec{r}) &= -\frac{\lambda}{2\mu_c a} \delta(r-a) \psi_c(\vec{r}) \quad (5.126) \end{aligned}$$

In order to compactify the formulas, let us define the following operators: H_c , which describes the confinement dynamics in the interaction region, H_f , which describes the dynamics of the scattered particles at large distances, and V_t , which describes the transition interaction. In configuration space we define those operators by

$$\begin{aligned} H_c &= -\frac{\nabla_r^2}{2\mu_c} + m_q + m_{\bar{q}} + \frac{1}{2}\mu_c\omega^2 r^2 \quad , \\ H_f &= -\frac{\nabla_r^2}{2\mu_f} + M_1 + M_2 \quad , \quad \text{and} \\ V_t &= \frac{\lambda}{2\mu_c a} \delta(r-a) \quad . \end{aligned} \quad (5.127)$$

Hence, we obtain for the wave equation

$$(E - H_c) \psi_c(\vec{r}) = V_t \psi_f(\vec{r}) \quad \text{and} \quad (E - H_f) \psi_f(\vec{r}) = [V_t]^T \psi_c(\vec{r}) \quad . \quad (5.128)$$

In the equations (5.128) we must eliminate ψ_c , since it is vanishing at large distances and thus *unobservable*. Formally, this can easily be done. We obtain then the following relation

$$\begin{aligned} \psi_f(\vec{r}) &= (E - H_f)^{-1} \{ [V_t]^T \psi_c(\vec{r}) \} \\ &= (E - H_f)^{-1} [V_t]^T (E - H_c)^{-1} V_t \psi_f(\vec{r}) \quad . \end{aligned} \quad (5.129)$$

By comparison of equation (5.129) with the usual expressions for the scattering wave equations, we must conclude that the generalized potential, V , is here given by

$$V = [V_t]^T (E - H_c)^{-1} V_t \quad . \quad (5.130)$$

The Born term

In the momentum representation formula (5.130) looks like

$$\langle \vec{p} | V | \vec{p}' \rangle = \langle \vec{p} | [V_t]^T (E - H_c)^{-1} V_t | \vec{p}' \rangle . \quad (5.131)$$

The properly normalized eigensolutions of the operator H_c (5.127) corresponding to the energy eigenvalue $E_{n\ell}$ are in configuration space given by

$$\langle \vec{r} | n\ell m \rangle = (\mu_c \omega)^{\frac{3}{4}} \mathcal{N}_{n\ell} Y_m^{(\ell)}(\hat{r}) \mathcal{F}_{n\ell}(\sqrt{\mu_c \omega} r) , \quad \text{where} \quad (5.132)$$

$$\mathcal{N}_{n\ell} = \sqrt{\left\{ \frac{2 \Gamma\left(n + \ell + \frac{3}{2}\right)}{n! \left[\Gamma\left(\ell + \frac{3}{2}\right)\right]^2} \right\}} \quad \text{and} \quad \mathcal{F}_{n\ell}(z) = z^\ell e^{-\frac{1}{2}z^2} {}_1F_1\left(-n; \ell + \frac{3}{2}; z^2\right) ,$$

$$E_{n\ell} = \omega \left(2n + \ell + \frac{3}{2}\right) + m_q + m_{\bar{q}} ,$$

and where $n = 0, 1, 2, \dots; \ell = 0, 1, 2, \dots; m = -\ell, \dots, +\ell$.

So, by letting the self-adjoint operator H_c act to the left, we may write

$$\begin{aligned} \langle \vec{p} | V | \vec{p}' \rangle &= \sum_{n\ell m} \langle \vec{p} | [V_t]^T | n\ell m \rangle \langle n\ell m | (E - H_c)^{-1} V_t | \vec{p}' \rangle \\ &= \sum_{n\ell m} \langle \vec{p} | [V_t]^T \frac{| n\ell m \rangle \langle n\ell m |}{E - E_{n\ell}} V_t | \vec{p}' \rangle . \end{aligned} \quad (5.133)$$

Next, we insert several times unity to obtain

$$\begin{aligned} \langle \vec{p} | V | \vec{p}' \rangle &= \sum_{n\ell m} \int d^3 r \int d^3 r'' \int d^3 r''' \int d^3 r' \\ &\frac{1}{E - E_{n\ell}} \langle \vec{p} | \vec{r} \rangle \langle \vec{r} | [V_t]^T | \vec{r}'' \rangle \langle \vec{r}'' | n\ell m \rangle \langle n\ell m | \vec{r}''' \rangle \langle \vec{r}''' | V_t | \vec{r}' \rangle \langle \vec{r}' | \vec{p}' \rangle . \end{aligned} \quad (5.134)$$

Two of the four integrations are trivial, since, as we have seen in section (5.1.1), the non-local equivalent of the local transition potential takes the form

$$\langle \vec{r} | V_t | \vec{r}' \rangle = \frac{\lambda}{2\mu_c a} \delta(r - a) \delta^{(3)}(\vec{r} - \vec{r}') . \quad (5.135)$$

By inserting expression (5.135) into formula (5.134) and also substituting

$$\langle \vec{r} | \vec{p} \rangle = \frac{e^{i\vec{p} \cdot \vec{r}}}{(2\pi)^{3/2}} , \quad (5.136)$$

we find

$$\begin{aligned}
\langle \vec{p} | V | \vec{p}' \rangle &= \sum_{n\ell m} \int d^3r \int d^3r' & (5.137) \\
&\frac{1}{E - E_{n\ell}} \frac{e^{-i\vec{p} \cdot \vec{r}}}{(2\pi)^{3/2}} \frac{\lambda}{2\mu_c a} \delta(r - a) \langle \vec{r} | n\ell m \rangle \\
&\langle n\ell m | \vec{r}' \rangle \frac{\lambda}{2\mu_c a} \delta(r' - a) \frac{e^{i\vec{p}' \cdot \vec{r}'}}{(2\pi)^{3/2}} .
\end{aligned}$$

Next, we observe that the radial parts of the two remaining integrations are also trivial, because of the two delta-functions. We insert thus two times the expression given in formula (5.132) for the harmonic oscillator eigenfunctions, to obtain

$$\begin{aligned}
\langle \vec{p} | V | \vec{p}' \rangle &= \frac{(\mu_c \omega)^{3/2}}{(2\pi)^3} \left(\frac{\lambda}{2\mu_c a} \right)^2 \sum_{n\ell m} \mathcal{N}_{n\ell}^2 a^2 \int d\Omega a^2 \int d\Omega' & (5.138) \\
&\frac{1}{E - E_{n\ell}} e^{-i\vec{p} \cdot a\hat{r}} Y_m^{(\ell)}(\hat{r}) \mathcal{F}_{n\ell}(\sqrt{\mu_c \omega} a) \\
&Y_m^{(\ell)*}(\hat{r}') \mathcal{F}_{n\ell}(\sqrt{\mu_c \omega} a) e^{i\vec{p}' \cdot a\hat{r}'} .
\end{aligned}$$

For the integrations over the angles we introduce Bauer's formula

$$e^{-i\vec{k} \cdot \vec{r}} = \sum_{\lambda, \mu} 4\pi (-i)^\lambda j_\lambda(kr) Y_\mu^{(\lambda)*}(\hat{r}) Y_\mu^{(\lambda)}(\hat{k}) , \quad (5.139)$$

for which we have no further reference then the remark at page 189 of the lecture notes [6] of J.J. de Swart, in order to obtain

$$\int d\Omega e^{-i\vec{p} \cdot a\hat{r}} X^{(0)}(\hat{r}) Y_m^{(\ell)}(\hat{r}) = 4\pi (-i)^\ell j_\ell(pa) Y_m^{(\ell)*}(\hat{p}) \quad (5.140)$$

and

$$\int d\Omega' e^{i\vec{p}' \cdot a\hat{r}'} X^{(0)*}(\hat{r}') Y_m^{(\ell)}(\hat{r}') = 4\pi (i)^\ell j_\ell(p'a) Y_m^{(\ell)}(\hat{p}') \quad (5.141)$$

Substitution of relations (5.140) and (5.141) into formula (5.138) gives us the following expression

$$\begin{aligned}
\langle \vec{p} | V | \vec{p}' \rangle &= \frac{\lambda^2 a^2 \omega}{2\pi} \sqrt{\frac{\omega}{\mu_c}} \sum_{n\ell m} \mathcal{N}_{n\ell}^2 & (5.142) \\
&\frac{1}{E - E_{n\ell}} Y_m^{(\ell)*}(\hat{p}) Y_m^{(\ell)}(\hat{p}') j_\ell(pa) j_\ell(p'a) \mathcal{F}_{n\ell}^2(\sqrt{\mu_c \omega} a) .
\end{aligned}$$

The summation over the magnetic quantum number m can be performed by the use of the addition theorem (see formula 5.22), to give

$$\begin{aligned}
\langle \vec{p} | V | \vec{p}' \rangle &= \tag{5.143} \\
&= \frac{\lambda^2 a^2 \omega}{2\pi} \sqrt{\frac{\omega}{\mu_c}} \sum_{nl} \mathcal{N}_{nl}^2 \frac{1}{E - E_{nl}} \frac{2\ell + 1}{4\pi} P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) j_\ell(p'a) \mathcal{F}_{nl}^2(\sqrt{\mu_c \omega} a) \\
&= \frac{\lambda^2 a^2 \omega}{8\pi^2} \sqrt{\frac{\omega}{\mu_c}} \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) j_\ell(p'a) \sum_{n=0}^{\infty} \frac{\mathcal{N}_{nl}^2 \mathcal{F}_{nl}^2(\sqrt{\mu_c \omega} a)}{E - E_{nl}} .
\end{aligned}$$

For the summation over the radial quantum number n the result may be looked up in [8] at page 227. Using the definition of \mathcal{A} which is given formula (5.113), one finds

$$\begin{aligned}
\langle \vec{p} | V | \vec{p}' \rangle &= \tag{5.144} \\
&= \frac{\lambda^2 a^2 \omega}{8\pi^2} \sqrt{\frac{\omega}{\mu_c}} \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\hat{p} \cdot \hat{p}') j_\ell(pa) j_\ell(p'a) \frac{-\Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{\omega \sqrt{\mu_c \omega a^2}} ,
\end{aligned}$$

where, following formulas (5.104) and (5.108), ν is related to p according to

$$p^2 = 2\mu_f \left[\omega \left(2\nu + \ell + \frac{3}{2} \right) + m_q + m_{\bar{q}} - M_1 - M_2 \right] . \tag{5.145}$$

The Born term (5.144) may be compared to the first order term of the result obtained in formula (5.114), which by means of formulas (5.19), (5.25) and (5.26), leads to

$$\begin{aligned}
T_\ell(p) &= -\frac{1}{4\pi^2 \mu_f p} \frac{1}{\cotg(\delta_\ell(p)) - i} \tag{5.146} \\
&= -\frac{1}{4\pi^2 \mu_f p} \frac{\frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} pa j_\ell^2(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{1 - i \frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} pa j_\ell(pa) h_\ell^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)} \\
&= -\frac{1}{8\pi^2 \mu_c} \frac{\lambda^2 a j_\ell^2(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{1 - i \frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} pa j_\ell(pa) h_\ell^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)} \\
&= -\frac{\lambda^2 a j_\ell^2(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{8\pi^2 \mu_c} \times \\
&\quad \times \left\{ 1 + i \frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} pa j_\ell(pa) h_\ell^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) + \right. \\
&\quad \left. + \left(i \frac{1}{2} \lambda^2 \frac{\mu_f}{\mu_c} pa j_\ell(pa) h_\ell^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2) \right)^2 + \dots \right\} .
\end{aligned}$$

We find perfect agreement.

The full matrix elements

For the higher order terms one needs paper and some patience. However, no further difficulties will emerge than already exposed here in this chapter. One obtains then

$$\begin{aligned}
 T(\vec{p}, \vec{p}') &= \tag{5.147} \\
 &= -\frac{\lambda^2 a}{8\pi^2 \mu_c} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') \frac{j_{\ell}(pa) j_{\ell}(p'a) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{1 - i\frac{1}{2}\lambda^2 \frac{\mu_f}{\mu_c} pa j_{\ell}(pa) h_{\ell}^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}
 \end{aligned}$$

Notice that the above expression (5.147) is indeed of the form (5.19). We may thus arrive at the scattering amplitude by substitution of the on-shell (*i.e.* $p' = p$) matrix elements in formula (5.25) by

$$T_{\ell}(p) = -\left(\frac{\lambda^2 a}{8\pi^2 \mu_c} \right) \frac{j_{\ell}^2(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)}{1 - i\frac{1}{2}\lambda^2 \frac{\mu_f}{\mu_c} pa j_{\ell}(pa) h_{\ell}^{(1)}(pa) \Gamma(-\nu) \mathcal{A}(\nu, \ell; \mu_c \omega a^2)} \quad , \tag{5.148}$$

which, by the use of formula (5.27), may be compared to expression (5.115).

Finally, it is interesting to study the limit $\lambda \rightarrow \infty$ in formula (5.147), *i.e.*

$$T(\vec{p}, \vec{p}') \xrightarrow{\lambda \rightarrow \infty} -\frac{i}{4\pi^2 \mu_f p} \sum_{\ell=0}^{\infty} (2\ell + 1) P_{\ell}(\hat{p} \cdot \hat{p}') \frac{j_{\ell}(p'a)}{h_{\ell}^{(1)}(pa)} \quad , \tag{5.149}$$

to notice, by comparison to formula (5.80), that this way we may obtain the expression for the T -matrix elements of the infinitely hard sphere. Indeed, in the limit of very large coupling (λ) the structure of the resonance channel ψ_c becomes invisible. What remains is the screening hard sphere.

Chapter 6

Relativistic kinematics

6.1 Relativistic kinematics

The total energy, E_{total} , for a system of two non-interacting on-mass-shell particles of masses m_1 and m_2 , which are freely moving with linear momenta respectively \vec{p}_1 and \vec{p}_2 , is given by the sum of the individual energies, $E(\vec{p}_1)$ and $E(\vec{p}_2)$ respectively, according to

$$E_{\text{total}} = E(\vec{p}_1) + E(\vec{p}_2) = \sqrt{\vec{p}_1^2 + m_1^2} + \sqrt{\vec{p}_2^2 + m_2^2} . \quad (6.1)$$

In the center-of-mass frame, where $\vec{p}_1 = -\vec{p}_2 = \vec{p}$, one has the following relations:

$$\begin{aligned} s &= (E_{\text{CM, total}})^2 = 2\vec{p}^2 + m_1^2 + m_2^2 + 2\sqrt{\vec{p}^2 + m_1^2}\sqrt{-\vec{p}^2 + m_2^2} , \\ (s - 2\vec{p}^2 - m_1^2 - m_2^2)^2 &= 4(\vec{p}^2 + m_1^2)(-\vec{p}^2 + m_2^2) , \\ 4s\vec{p}^2 &= s^2 - 2s(m_1^2 + m_2^2) + m_1^4 + m_2^4 - 2m_1^2m_2^2 , \\ \text{and } \vec{p}^2 &= \frac{1}{4s} \left\{ [s - (m_1 + m_2)^2] [s - (m_1 - m_2)^2] \right\} . \end{aligned} \quad (6.2)$$

The Mandelstam variables, s , t and u , for the process

$$1 + 2 \longrightarrow 3 + 4 \quad (6.3)$$

are defined by

$$s = (p_1 + p_2)^2 , \quad t = (p_1 - p_3)^2 , \quad u = (p_1 - p_4)^2 , \quad (6.4)$$

or, alternatively, by using total four-momentum conservation which is given by

$$p_1 + p_2 = p_3 + p_4 , \quad (6.5)$$

one also has

$$s = (p_3 + p_4)^2 , \quad t = (p_2 - p_4)^2 , \quad u = (p_2 - p_3)^2 , \quad (6.6)$$

Notice that we use here the metric $(+, -, -, -)$, which for s gives

$$s = (p_1 + p_2)^2 = (E(\vec{p}_1) + E(\vec{p}_2))^2 - (\vec{p}_1 + \vec{p}_2)^2 . \quad (6.7)$$

In the the center-of-mass frame, where $\vec{p}_1 = -\vec{p}_2$, one obtains, moreover

$$s = (E(\vec{p}_1) + E(\vec{p}_2))^2 = (E_{\text{CM}})^2 , \quad (6.8)$$

which equals the total invariant mass, as already anticipated in formula (6.2).

Furthermore, from their definition one observes that the Mandelstam variables (6.4) are Lorentz invariant and hence invariants with respect to any Lorentz transformation.

By total momentum conservation 6.5, one deduces

$$\begin{aligned} s + t + u &= 3p_1^2 + p_2^2 + p_3^2 + p_4^2 + 2p_1 \cdot (p_2 - p_3 - p_4) \\ &= 3p_1^2 + p_2^2 + p_3^2 + p_4^2 - 2p_1^2 \\ &= p_1^2 + p_2^2 + p_3^2 + p_4^2 \\ &= m_1^2 + m_2^2 + m_3^2 + m_4^2 . \end{aligned} \quad (6.9)$$

Consequently, for on-mass-shell processes s , t and u are not independent.

In Fig. 6.1 we visualize things for the center-of-mass frame.

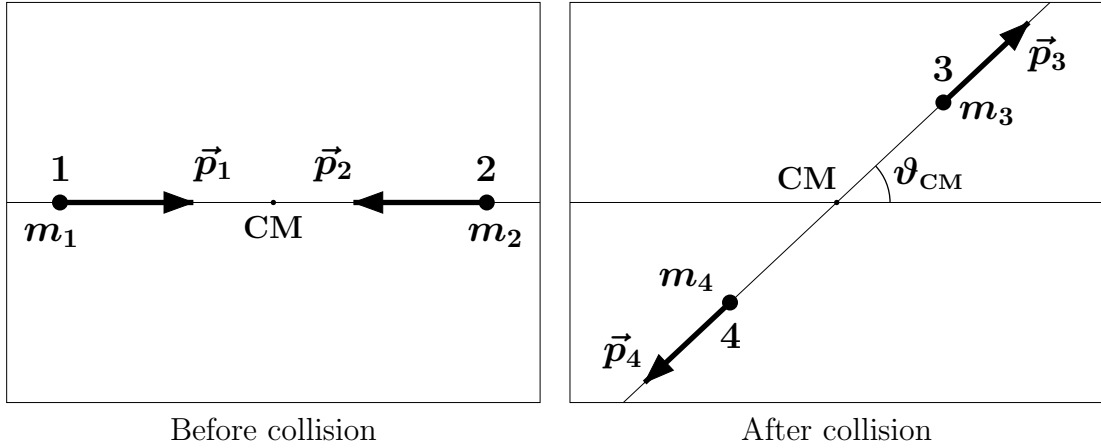


Figure 6.1: Collision in the center-of-mass system. Before collision particle 1 and particle 2 move towards their center of mass with equal and opposite three-momenta, \vec{p}_1 and \vec{p}_2 respectively. After collision particle 3 and particle 4 move away from their center of mass with equal and opposite three-momenta, \vec{p}_3 and \vec{p}_4 respectively.

The angle between the direction of motion of the outgoing particle 3 and the direction of motion of the incoming particle 1 is defined as the angle ϑ_{CM} of the scattering process of formula (6.3) in the center-of-mass system. It has the following relation with the Mandelstam variable t .

$$\begin{aligned} t &= (p_1 - p_3)^2 \\ &= (p_1)^2 + (p_3)^2 - 2p_1 \cdot p_3 \\ &= (p_1)^2 + (p_3)^2 - 2E(\vec{p}_1)E(\vec{p}_3) + 2\vec{p}_1 \cdot \vec{p}_3 \\ &= (m_1)^2 + (m_3)^2 - 2\sqrt{(\vec{p}_1)^2 + (m_1)^2}\sqrt{(\vec{p}_3)^2 + (m_3)^2} + 2|\vec{p}_1||\vec{p}_3|\cos(\vartheta_{\text{CM}}) . \end{aligned} \quad (6.10)$$

6.1.1 $\pi^+ \pi^- \rightarrow K^+ K^{*-}$

Consider a π^+ meson which annihilates with a π^- meson, resulting in two outgoing Kaon mesons, a K^+ meson and a K^{*-} meson. The π^- meson is at rest in the laboratory, whereas the π^+ meson has a total energy of 9.0 GeV. The Kaon meson comes out with an angle of 60° with respect to the direction of the incoming pion, in the center-of-mass system.

Given this information, we may determine the other kinematical quantities. For the masses of the particles we take

$$m_\pi = 0.14 \text{ GeV} \quad , \quad m_K = 0.50 \text{ GeV} \quad , \quad m_{K^*} = 0.89 \text{ GeV} \quad .$$

Let us first determine the total invariant mass of the system.

$$\sqrt{s} = \sqrt{2m_\pi^2 + 2E_{\pi^+}m_\pi} = 1.60 \text{ GeV} \quad .$$

With that result we may determine \vec{p}_π^2 in the center-of-mass frame.

$$(\vec{p}_\pi)^2 = \frac{1}{4} [s - 4m_\pi^2] = 0.62 \text{ (GeV)} \quad .$$

Next, we can determine $(\vec{p}_K)^2$ in the center-of-mass frame, as follows

$$(\vec{p}_K)^2 = \frac{1}{4s} \left\{ [s - (m_K + m_{K^*})^2] [s - (m_K - m_{K^*})^2] \right\} = 0.148 \text{ (GeV)} \quad .$$

The linear momentum of K^* is in the center-of-mass frame opposite to \vec{p}_K , of course. Consequently, we can check our calculations by determining the total invariant mass \sqrt{s} after collision. This gives

$$\sqrt{s} = \sqrt{\vec{p}_K^2 + m_K^2} + \sqrt{\vec{p}_{K^*}^2 + m_{K^*}^2} = 0.63 \text{ (GeV)} + 0.97 \text{ (GeV)} = 1.6 \text{ (GeV)} \quad ,$$

which is indeed what we obtained for the situation before collision.

Then we may determine t and u

$$t = (m_\pi)^2 + (m_K)^2 - 2E_\pi E_K + 2|\vec{p}_\pi| |\vec{p}_K| \cos(\vartheta_{\text{CM}}) = -0.437 \text{ GeV}^2 \quad .$$

and

$$u = (m_\pi)^2 + (m_{K^*})^2 - 2E_\pi E_{K^*} + 2|\vec{p}_\pi| |\vec{p}_{K^*}| \cos(\pi - \vartheta_{\text{CM}}) = -1.04 \text{ GeV}^2 \quad .$$

We will denote the total momentum of a particle in the laboratory by q and its linear momentum by \vec{q} . The π^- meson is at rest, hence $\vec{q}_{\pi^-} = 0$. For the π^+ we have

$$E(\vec{q}_{\pi^+}) = \sqrt{(\vec{q}_{\pi^+})^2 + m_{\pi^+}^2} = 9 \text{ (GeV)} \quad \Longleftrightarrow \quad \vec{q}_{\pi^+} \approx 9 \text{ (GeV)} \quad .$$

Moreover, since $\vec{q}_{\pi^-} = 0$, we have for t the relation

$$t = (q_{\pi^-} - q_{K^*})^2 = m_{\pi^-}^2 + m_{K^*}^2 - 2m_{\pi^-} \sqrt{\vec{q}_{K^*}^2 + m_{K^*}^2} \quad ,$$

hence

$$\vec{q}_{K^*}^2 = \left(\frac{m_{\pi^-}^2 + m_{K^*}^2 - t}{2m_{\pi^-}} \right)^2 - m_{K^*}^2 = 4.37 \text{ GeV}^2 \quad .$$

Similarly

$$u = (q_{\pi^-} - q_K)^2 = m_{\pi^-}^2 + m_K^2 - 2m_{\pi^-} \sqrt{\vec{q}_K^2 + m_K^2} \quad ,$$

hence

$$\vec{q}_K^2 = \left(\frac{m_{\pi^-}^2 + m_K^2 - u}{2m_{\pi^-}} \right)^2 - m_K^2 = 4.66 \text{ GeV}^2 \quad .$$

Also

$$E(\vec{q}_K) = \sqrt{\vec{q}_K^2 + m_K^2} = 4.68 \text{ (GeV)} \quad ,$$

and

$$E(\vec{q}_{K^*}) = \sqrt{\vec{q}_{K^*}^2 + m_{K^*}^2} = 4.46 \text{ (GeV)} \quad .$$

Finally, we determine the angle in the frame of the laboratory, of the direction of the outgoing K meson with respect to the direction of the incoming π^+ meson.

$$\cos(\theta_{K,\text{lab}}) = \frac{t - m_{\pi^+}^2 - m_K^2 + 2E(\vec{q}_{\pi^+})E(\vec{q}_K)}{2|\vec{q}_{\pi^+}||\vec{q}_K|} = 0.9974 \quad ,$$

corresponding to an angle of 4.1 degrees.

6.1.2 Elastic Scattering in the center-of-mass system

In elastic scattering the outgoing particles are identical to the incoming particles, which at this level amounts to $m_3 = m_1$ and $m_4 = m_2$. When we define the three-momenta before and after collision by respectively \vec{p} and \vec{p}' , then we have

$$\vec{p}_1 = -\vec{p}_2 = \vec{p} \quad \text{and} \quad \vec{p}_3 = -\vec{p}_4 = \vec{p}' \quad , \quad (6.11)$$

hence, by using formula (6.2),

$$\begin{aligned} \vec{p}^2 &= \frac{1}{4s} \left\{ [s - (m_1 + m_2)^2] [s - (m_1 - m_2)^2] \right\} \\ \text{and } \vec{p}'^2 &= \frac{1}{4s} \left\{ [s - (m_3 + m_4)^2] [s - (m_3 - m_4)^2] \right\} \quad . \end{aligned} \quad (6.12)$$

Since, moreover, $m_3 = m_1$ and $m_4 = m_2$ for elastic scattering, we have for the center-of-mass three-momenta in that case

$$\vec{p}^2 = \vec{p}'^2 \quad . \quad (6.13)$$

Substitution of the result (6.13) in expressions (6.8) and (6.10) gives the results

$$\begin{aligned} s &= \left(\sqrt{(\vec{p})^2 + (m_1)^2} + \sqrt{(\vec{p})^2 + (m_2)^2} \right)^2 \\ &= (\vec{p})^2 + (m_1)^2 + (\vec{p})^2 + (m_2)^2 + 2\sqrt{(\vec{p})^2 + (m_1)^2} \sqrt{(\vec{p})^2 + (m_2)^2} \\ &= 2(\vec{p})^2 + (m_1)^2 + (m_2)^2 + 2\sqrt{(\vec{p})^2 + (m_1)^2} \sqrt{(\vec{p})^2 + (m_2)^2} \quad , \end{aligned} \quad (6.14)$$

and

$$\begin{aligned}
t &= (m_1)^2 + (m_3)^2 - 2\sqrt{\vec{p}^2 + (m_1)^2}\sqrt{\vec{p}'^2 + (m_3)^2} + 2|\vec{p}'|\cos(\vartheta_{\text{CM}}) \\
&= 2(m_1)^2 - 2(\vec{p}^2 + (m_1)^2) + 2\vec{p}^2 \cos(\vartheta_{\text{CM}}) \\
&= 2\vec{p}^2 \{-1 + \cos(\vartheta_{\text{CM}})\} \quad . \quad (6.15)
\end{aligned}$$

Furthermore

$$\begin{aligned}
u &= (m_1)^2 + (m_4)^2 - 2\sqrt{\vec{p}^2 + (m_1)^2}\sqrt{\vec{p}'^2 + (m_4)^2} + 2\vec{p}_1 \cdot \vec{p}_4 \\
&= (m_1)^2 + (m_2)^2 - 2\sqrt{(\vec{p})^2 + (m_1)^2}\sqrt{(\vec{p}')^2 + (m_2)^2} - 2\vec{p}^2 \cos(\vartheta_{\text{CM}}) \quad . \quad (6.16)
\end{aligned}$$

As is obvious from the definitions of ϑ_{CM} in Fig. 6.1 and \vec{p} in formula (6.11), one has

$$\vec{p}^2 \geq 0 \quad \text{and} \quad -1 \leq \cos(\vartheta_{\text{CM}}) \leq +1 \quad , \quad (6.17)$$

hence for the Mandelstam variables s (formula 6.14) and t (formula 6.15), we find

$$s \geq (m_1 + m_2)^2 \quad \text{and} \quad t \leq 0 \quad . \quad (6.18)$$

6.1.3 Elastic Scattering in the lab system

In the laboratory system particle 2 is assumed to be at rest. This is visualized in Fig. 6.2. We define the laboratory four-momenta by q_1, q_2, q_3 and q_4 , in order to distinguish from the center-of-mass four-momenta. We study here again the case of elastic scattering, which implies $m_3 = m_1$ and $m_4 = m_2$.

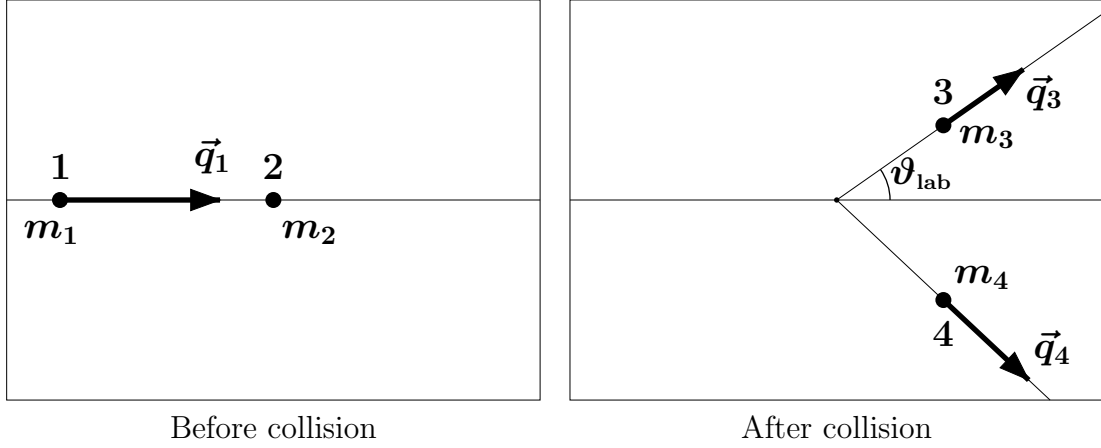


Figure 6.2: Collision in the laboratory system. Before collision particle 1 moves with three-momentum \vec{q}_1 towards particle 2 at rest ($\vec{q}_2 = 0$) in the center of coordinates. After collision particle 3 and particle 4 move away from the center of coordinates with three-momenta \vec{q}_3 and \vec{q}_4 respectively.

Here, we obtain for the Mandelstam variables (6.4), which, as mentioned before, are invariant under Lorentz transformations, hence the same for the laboratory system and the center-of-mass system,

$$\begin{aligned}
 s &= (q_1 + q_2)^2 = (m_1)^2 + (m_2)^2 + 2E(\vec{q}_1)E(\vec{q}_2) - 2\vec{q}_1 \cdot \vec{q}_2 \\
 &= (m_1)^2 + (m_2)^2 + 2E(\vec{q}_1)m_2 \\
 t &= (q_1 - q_3)^2 = 2(m_1)^2 - 2E(\vec{q}_1)E(\vec{q}_3) + 2\vec{q}_1 \cdot \vec{q}_3 \\
 &= 2(m_1)^2 - 2E(\vec{q}_1)E(\vec{q}_3) + 2|\vec{q}_1||\vec{q}_3|\cos(\vartheta_{\text{lab}}) \\
 u &= (q_2 - q_3)^2 = (m_1)^2 + (m_2)^2 - 2m_2E(\vec{q}_3) \quad .
 \end{aligned} \tag{6.19}$$

Also using formula (6.9), we find for t

$$t = 2m_1 + 2m_2 - s - u = 2m_2(E(\vec{q}_3) - E(\vec{q}_1)) \quad . \tag{6.20}$$

One defines the kinetic energy of the incoming particle by

$$T_1 = E(\vec{q}_1) - m_1 \quad . \tag{6.21}$$

At threshold, where $\vec{q}_1 = 0$, we obtain $T_1 = 0$.

6.1.4 Scattering in the forward direction

When \vec{q}_3 is in the forward direction, *i.e.* $\vartheta_{\text{lab}} = \vartheta_{\text{CM}} = 0$, it has no transversal component. Hence, by total three-momentum conservation also \vec{q}_4 is in the longitudinal direction. Furthermore, because of result (6.13), we have

$$\vec{p}_1 = \vec{p}_3 \quad . \quad (6.22)$$

As a consequence, also using formula (6.4)

$$t = (p_1 - p_3)^2 = (E(\vec{p}_1) - E(\vec{p}_3))^2 - (\vec{p}_1 - \vec{p}_3)^2 = 0 \quad . \quad (6.23)$$

Furthermore, we define the variable ν

$$\nu = \frac{s - u}{4m_2} = \frac{E(\vec{q}_1) + E(\vec{q}_3)}{2} = E(\vec{q}_1) + \frac{t}{4m_2} \quad , \quad (6.24)$$

also using formulae (6.19) and (6.20). For scattering in the forward direction, where $t = 0$, the variable ν represents the total energy of the incoming particle in the laboratory system.

Notice that, because of total four-momentum conservation, one has

$$\begin{aligned} s - u &= (p_1 + p_2)^2 - (p_1 - p_4)^2 = (p_1 + p_2) \cdot (p_3 + p_4) - (p_1 - p_4) \cdot (p_3 - p_2) = \\ &= p_1 \cdot p_4 + p_2 \cdot p_3 + p_1 \cdot p_2 + p_4 \cdot p_3 = (p_1 + p_3) \cdot (p_2 + p_4) \quad , \end{aligned}$$

hence

$$\nu = \frac{s - u}{4m_2} = \frac{(p_1 + p_3) \cdot (p_2 + p_4)}{4m_2} \quad . \quad (6.25)$$

6.2 Crossing

In the following we study the elastic scattering of two different processes. In the first process one scatters two particles a and b , whereas in the second process the antiparticle \bar{a} is scattered with b . The four-momentum of the incoming antiparticle \bar{a} in the second process is chosen opposite to the four-momentum of the outgoing particle a in the first process, and vice-versa, *i.e.*

$$\begin{aligned} a(p_1) + b(p_2) &\longrightarrow a(p_3) + b(p_4) & \text{(I)} \\ \bar{a}(-p_3) + b(p_2) &\longrightarrow \bar{a}(-p_1) + b(p_4) & \text{(II)} \end{aligned} \quad (6.26)$$

It can be shown that the scattering-matrix elements for the two processes are equal. Consequently, this represents a symmetry of the dynamical equations, which is called *crossing symmetry*.

Here, it is of interest to compare the Mandelstam variables of the two processes. From formula (6.4) we find for the first process

$$s_{\text{I}} = (p_1 + p_2)^2 \quad , \quad t_{\text{I}} = (p_1 - p_3)^2 \quad , \quad u_{\text{I}} = (p_1 - p_4)^2 \quad , \quad (6.27)$$

whereas for the second process, also using formula (6.6), we find

$$s_{\text{II}} = (-p_1 + p_4)^2 \quad , \quad t_{\text{II}} = (-p_1 + p_3)^2 \quad , \quad u_{\text{II}} = (p_2 + p_1)^2 \quad . \quad (6.28)$$

From formulae (6.27) and (6.28) we observe that the roles of s and u are interchanged

$$s_{\text{II}} = u_{\text{I}} \quad , \quad t_{\text{II}} = t_{\text{I}} \quad , \quad u_{\text{II}} = s_{\text{I}} \quad , \quad (6.29)$$

for process (6.26,II) with respect to process (6.26,I). One says the the process (6.26,II) is represented by the u -channel of process (6.26,I).

Observe, moreover, that for the variable ν which has been defined in formula (6.24), we have

$$\nu_{\text{II}} = -\nu_{\text{I}} \quad . \quad (6.30)$$

6.3 The physical region for elastic scattering

The variables ν and t are related to the variables \vec{p}^2 and ϑ_{CM} as can be seen from expressions (6.24) and (6.15). Physically allowed values for \vec{p}^2 and ϑ_{CM} are given by

$$\vec{p}^2 \geq 0 \quad \text{and} \quad -1 \leq \cos(\vartheta_{\text{CM}}) \leq +1 \quad . \quad (6.31)$$

Hence, it has to be expected that for related variables the physical region, *i.e.* the region of allowed physical values, is also restricted. Furthermore, \vec{p}^2 and ϑ_{CM} are rather independent. But, the dependence of ν and t is not very clear from their definitions.

In formula (6.18) we indicate the physical limits for the Mandelstam variables s and t in the case of elastic scattering, *i.e.* $m_3 = m_1$ and $m_4 = m_2$. Here we will study this subject in more detail, moreover concentrating on the variables ν and t .

From equation (6.13) we learn that for elastic on-shell scattering one has for the total energies of the four particles involved

$$E(\vec{p}_3) = E(\vec{p}_1) \quad \text{and} \quad E(\vec{p}_4) = E(\vec{p}_2) \quad . \quad (6.32)$$

We will frequently use the relations (6.13) and (6.32) in the following.

From the expressions (6.14), (6.16) and the definition of ν , which is given in formula (6.24), we deduce

$$\nu = \frac{1}{m_2} \left[E(\vec{p}_1) E(\vec{p}_2) + \frac{1}{2} \vec{p}^2 \{1 + \cos(\vartheta_{\text{CM}})\} \right] \quad . \quad (6.33)$$

Except for the forward direction where $\cos(\vartheta_{\text{CM}}) = 1$, we may use expression (6.15) in order to substitute \vec{p}^2 for t .

$$\nu = \quad (6.34)$$

$$\frac{1}{m_2} \left[\sqrt{(m_1)^2 - \frac{t}{2\{1 - \cos(\vartheta_{\text{CM}})\}}} \sqrt{(m_2)^2 - \frac{t}{2\{1 - \cos(\vartheta_{\text{CM}})\}}} - \frac{t\{1 + \cos(\vartheta_{\text{CM}})\}}{4\{1 - \cos(\vartheta_{\text{CM}})\}} \right] \quad .$$

Furthermore, in the forward direction we have

$$t = 0 \quad \text{and} \quad \nu = \frac{1}{m_2} \left[E(\vec{p}_1) E(\vec{p}_2) + \vec{p}^2 \right] \geq m_1 \quad . \quad (6.35)$$

From formula (6.34) we observe that a condition for ν being real, is given by

$$t \leq (m_1)^2 \{1 - \cos(\vartheta_{\text{CM}})\} \quad \text{or} \quad t \leq (m_2)^2 \{1 - \cos(\vartheta_{\text{CM}})\} \quad , \quad (6.36)$$

depending on whether $m_1 < m_2$, or $m_1 > m_2$. Let us assume that $m_1 < m_2$. In that case we find that for ν to be real, t can at most equal $4(m_1)^2$. However, this value is outside the physical region, because of condition (6.18). Consequently, t can take any value from $t = 0$ to $t = -\infty$ in the physical region, as is expressed by relation (6.15). The related physical values of ν can be found from formulas (6.34) and (6.35), by varying $\cos(\vartheta_{\text{CM}})$ within the limits (6.31).

In order to make some graphical representations of the various formulas, we will concentrate now on πN elastic scattering. In figure (6.3) we have depicted the situation. The physical region for ν and t in the s -channel process given in formula (6.3), is shaded. The

upper boundary is given by $t = 0$, corresponding to forward scattering, whereas the lower boundary, corresponding to backward scattering, is given by

$$\nu = \frac{1}{m_2} \sqrt{(m_1)^2 - \frac{t}{4}} \sqrt{(m_2)^2 - \frac{t}{4}}. \quad (6.37)$$

We have chosen here $m_1 = 0.14$ GeV and $m_2 = 0.94$, which corresponds to πN elastic scattering. The solid lines correspond to constant values for ϑ_{CM} .

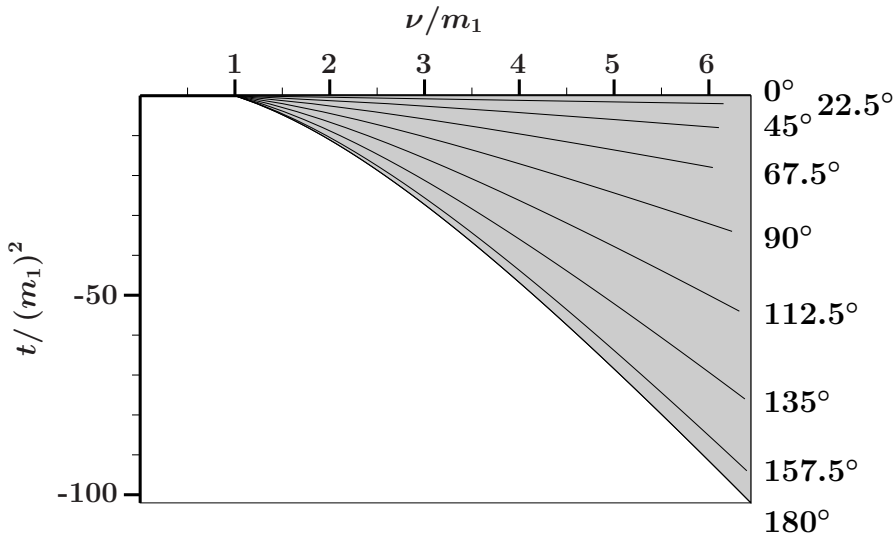


Figure 6.3: Elastic s -channel πN scattering ($m_1 = m_\pi = 0.14$ GeV, $m_2 = m_N = 0.94$ GeV). The shaded area, which is understood to extend to infinity, represents the physically allowed region for ν and t . The solid lines result from formula (6.34) for constant ϑ_{CM} , the values of which are indicated on the righthand side of the figure.

Once an amplitude, or any other physical quantity, is determined in terms of the variables ν and t , one can in principle extend the values of those variables to outside the physical region. Such procedure is sometimes advantageous, for example when the amplitude has a zero for a certain set of values of those variables. In the latter case one may then Taylor expand the amplitude in a small region around that zero value and determine the first few coefficients of the expansion. When from experiment one has enough information to achieve an extension of fitted formulas to the same region, one may then compare models with "experiment" in the unphysical region. Now at this point we must notice that we can obtain a better performance of experiment if we could join knowledge of different regions. For that reason we come back here on the issue of crossing, which is discussed in section (6.2).

We have seen in formulae (6.29) and (6.30) that antipion-nucleon scattering is described by interchanging the roles of s and u , or equivalently by substituting ν by $-\nu$ in the expression of the amplitude. Consequently, the physical regions for the processes antipion-nucleon and pion-nucleon are each other mirror images, reflected around the t axis, as is represented in figure (6.4).

Now, since the π^0 is its own antiparticle, and the π^- is the antiparticle of the π^+ , pions and antipions are the same particles. Hence, both physical regions represented in figure (6.4), describe πN elastic scattering. Consequently, we may obtain experimental

knowledge of the scattering amplitudes for elastic πN scattering in both regions at the same time.

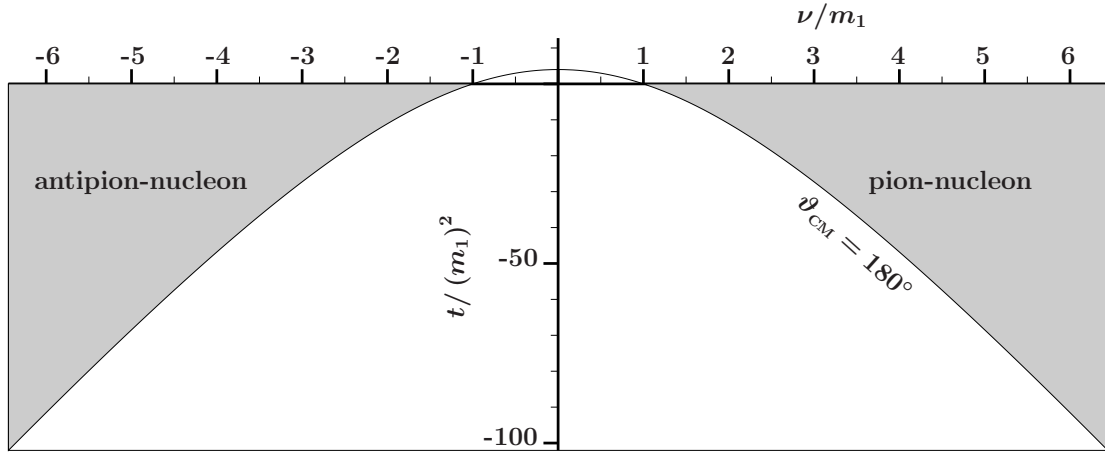


Figure 6.4: The physically allowed regions (shaded and assumed to extend to infinity), for pion-nucleon and for antipion-nucleon elastic scattering.

In figure (6.5) we show how the continuation of the curve for $\vartheta_{\text{CM}} = 180^\circ$ to values outside the physical region, include the combination $\nu = 0$ and $t = 4(m_1)^2$. The region

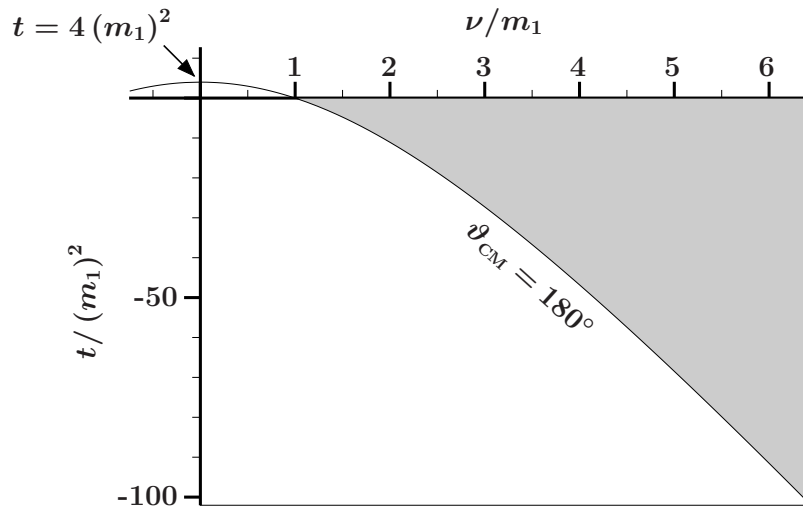


Figure 6.5: The combination $\nu = 0$ and $t = 4(m_1)^2$ lies on the continuation of the curve for $\vartheta_{\text{CM}} = 180^\circ$ to outside the physical region.

between the axis $t = 0$ for $-1 \leq \nu/m_1 \leq +1$ and the curve $\cos(\vartheta_{\text{CM}}) = -1$ is called the *subthreshold crescent* for πN elastic scattering. It is an unphysical region. But, experiment can be analytically continued into it from both sides.

6.3.1 The subthreshold crescent

In figure (6.6) we show in some detail the subthreshold crescent for πN elastic scattering. This nonphysical region touches the two physical regions for πN elastic scattering in the

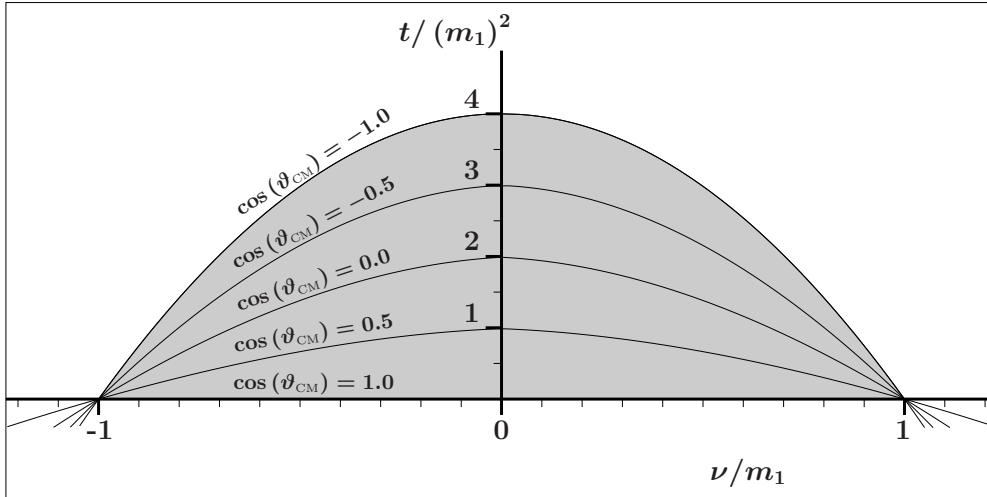


Figure 6.6: The region spanned by the line element $-1 \leq \nu \leq +1$ at the $t = 0$ axis and the curve given by the relation of formula (6.34) over the same interval for $\vartheta_{CM} = 180^\circ$, is shown here, as well as some curves for constant $\cos(\vartheta_{CM})$.

positions ($\nu = -1, t = 0$) and ($\nu = +1, t = 0$). The solid lines in figure (6.6) represent the curves for constant $\cos(\vartheta_{CM})$ at the values 1 (forward scattering), 1/2, 0 (transversal scattering), -1/2 and -1 (backward scattering). The curves seem to cross the line $\nu = 0$ at $t = 2(m_1)^2 \{1 - \cos(\vartheta_{CM})\}$. However, except for forward and backward scattering, this is only approximately true because of the smallness of the pion mass with respect to the nucleon mass, as can be observed from formula (6.34).

6.4 The amplitude for elastic πN scattering

Pions have isospin $I_\pi = 1$ and nucleons $I_N = \frac{1}{2}$. Consequently, the total isospin of the πN system may be $I_{\pi N} = \frac{1}{2}$ or $I_{\pi N} = \frac{3}{2}$. The related non-trivial Clebsch-Gordon coefficients $\langle I, I_z | \pi N \rangle$ are given by

$$\begin{aligned} \left\langle \frac{3}{2}, \frac{1}{2} \middle| \pi^+ n \right\rangle &= \left\langle \frac{3}{2}, -\frac{1}{2} \middle| \pi^- p \right\rangle = \sqrt{\frac{1}{3}} \ , \\ \left\langle \frac{3}{2}, \frac{1}{2} \middle| \pi^0 p \right\rangle &= \left\langle \frac{3}{2}, -\frac{1}{2} \middle| \pi^0 n \right\rangle = \sqrt{\frac{2}{3}} \ , \\ \left\langle \frac{1}{2}, \frac{1}{2} \middle| \pi^+ n \right\rangle &= -\left\langle \frac{1}{2}, -\frac{1}{2} \middle| \pi^- p \right\rangle = \sqrt{\frac{2}{3}} \ , \\ \text{and} \quad -\left\langle \frac{1}{2}, \frac{1}{2} \middle| \pi^0 p \right\rangle &= \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \pi^0 n \right\rangle = \sqrt{\frac{1}{3}} \ . \end{aligned} \quad (6.38)$$

Using the values of table (6.38) we obtain for instance

$$\begin{aligned} \left| I = \frac{3}{2}, I_z = -\frac{1}{2} \right\rangle &= \sqrt{\frac{1}{3}} \left| \pi^- p \right\rangle + \sqrt{\frac{2}{3}} \left| \pi^0 n \right\rangle \\ \text{and} \quad \left| I = \frac{1}{2}, I_z = -\frac{1}{2} \right\rangle &= -\sqrt{\frac{2}{3}} \left| \pi^- p \right\rangle + \sqrt{\frac{1}{3}} \left| \pi^0 n \right\rangle \ , \end{aligned} \quad (6.39)$$

for which the inverse relations are

$$\begin{aligned} \left| \pi^0 n \right\rangle &= \sqrt{\frac{1}{3}} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \sqrt{\frac{2}{3}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \text{and} \quad \left| \pi^- p \right\rangle &= \sqrt{\frac{2}{3}} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \ . \end{aligned} \quad (6.40)$$

Hence, the transition-matrix element for the process $\pi^- p \rightarrow \pi^0 n$ yields

$$\begin{aligned} \langle \pi^0 n | T | \pi^- p \rangle &= \\ &= \left\{ \sqrt{\frac{1}{3}} \left\langle \frac{3}{2}, -\frac{1}{2} \middle| - \sqrt{\frac{2}{3}} \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \right\} T \left\{ \sqrt{\frac{2}{3}} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \right\} \right. \\ &= \frac{\sqrt{2}}{3} \left\langle \frac{3}{2}, -\frac{1}{2} \middle| T \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \frac{1}{3} \left\langle \frac{3}{2}, -\frac{1}{2} \middle| T \left| \frac{1}{2}, -\frac{1}{2} \right\rangle + \right. \\ &\quad \left. - \frac{2}{3} \left\langle \frac{1}{2}, -\frac{1}{2} \middle| T \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \frac{\sqrt{2}}{3} \left\langle \frac{1}{2}, -\frac{1}{2} \middle| T \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \right. \ . \end{aligned} \quad (6.41)$$

When, furthermore, we assume that the operator T conserves isospin, then the transition-matrix elements for states with different total isospin must vanish. Hence, in that case

$$\langle \pi^0 n | T | \pi^- p \rangle = \frac{\sqrt{2}}{3} \left\{ \left\langle \frac{3}{2}, -\frac{1}{2} \middle| T \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left\langle \frac{1}{2}, -\frac{1}{2} \middle| T \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \right\} \ . \quad (6.42)$$

Moreover, strong interactions are independent of the isospin z component. Consequently, we may define

$$T^{(\frac{1}{2})} = \left\langle \frac{1}{2}, +\frac{1}{2} \middle| T \left| \frac{1}{2}, +\frac{1}{2} \right\rangle = \left\langle \frac{1}{2}, -\frac{1}{2} \middle| T \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \ , \quad (6.43)$$

and, similarly,

$$T^{(\frac{3}{2})} = \left\langle \frac{3}{2}, \pm \frac{3}{2} \left| T \right| \frac{3}{2}, \pm \frac{3}{2} \right\rangle = \left\langle \frac{3}{2}, \pm \frac{1}{2} \left| T \right| \frac{3}{2}, \pm \frac{1}{2} \right\rangle . \quad (6.44)$$

For the transition-matrix element (6.42) of the process $\pi^- p \rightarrow \pi^0 n$, we obtain then

$$\langle \pi^0 n | T | \pi^- p \rangle = \frac{\sqrt{2}}{3} \left\{ T^{(\frac{3}{2})} - T^{(\frac{1}{2})} \right\} . \quad (6.45)$$

The transition-matrix elements collected in table (6.1) are obtained following similar gymnastics for the other πN channels.

process	transition-matrix element
$\langle \pi^+ p T \pi^+ p \rangle = \langle \pi^- n T \pi^- n \rangle$	$T^{(\frac{3}{2})}$
$\langle \pi^+ n T \pi^+ n \rangle = \langle \pi^0 n T \pi^0 n \rangle$	$\frac{1}{3} \left\{ T^{(\frac{3}{2})} + 2T^{(\frac{1}{2})} \right\}$
$\langle \pi^- p T \pi^- p \rangle = \langle \pi^0 p T \pi^0 p \rangle$	$\frac{1}{3} \left\{ 2T^{(\frac{3}{2})} + T^{(\frac{1}{2})} \right\}$
$\langle \pi^0 n T \pi^- p \rangle = \langle \pi^0 p T \pi^+ n \rangle$	$\frac{\sqrt{2}}{3} \left\{ T^{(\frac{3}{2})} - T^{(\frac{1}{2})} \right\}$

Table 6.1: πN processes

6.4.1 The t channel

In section (6.2) we study $s \leftrightarrow u$ crossing. Here we will pay attention to the interchange of s and t . Thereto, we study the process

$$a(p_1) + \bar{a}(-p_3) \longrightarrow \bar{b}(-p_2) + b(p_4) \quad (\text{III}) \quad . \quad (6.46)$$

The Mandelstam variables (6.4) for the process (6.46) are given by

$$s_{\text{III}} = (p_1 - p_3)^2 = t_{\text{I}} \quad , \quad t_{\text{III}} = (p_1 + p_2)^2 = s_{\text{I}} \quad , \quad u_{\text{III}} = (p_1 - p_4)^2 = u_{\text{I}} \quad , \quad (6.47)$$

where s_{I} , t_{I} and u_{I} are defined in formula (6.27).

For πN elastic scattering, the process (6.46) represent the inelastic process

$$\pi\pi \longrightarrow \bar{N}N \quad . \quad (6.48)$$

The physical region for the process (6.48) is given by

$$t = t_{\text{I}} = s_{\text{III}} \geq (2m_N)^2 \quad , \quad s = s_{\text{I}} = t_{\text{III}} \leq 0 \quad . \quad (6.49)$$

In order to account for the condition (6.49) on t , we rewrite expression (6.34) in the following form.

$$\nu = \frac{1}{m_2} \left[\sqrt{\frac{t}{2\{1 - \cos(\vartheta_{\text{CM}})\}} - (m_1)^2} \sqrt{\frac{t}{2\{1 - \cos(\vartheta_{\text{CM}})\}} - (m_2)^2} - \frac{t\{1 + \cos(\vartheta_{\text{CM}})\}}{4\{1 - \cos(\vartheta_{\text{CM}})\}} \right] \quad (6.50)$$

The envelope of the physical region in the t channel is given by $\vartheta_{\text{CM}} = 180^\circ$, as in the case of the s channel and the u channel (see figures 6.3 and 6.4). In figure (6.7) we depict the three physical regions in the (ν, t) plane.

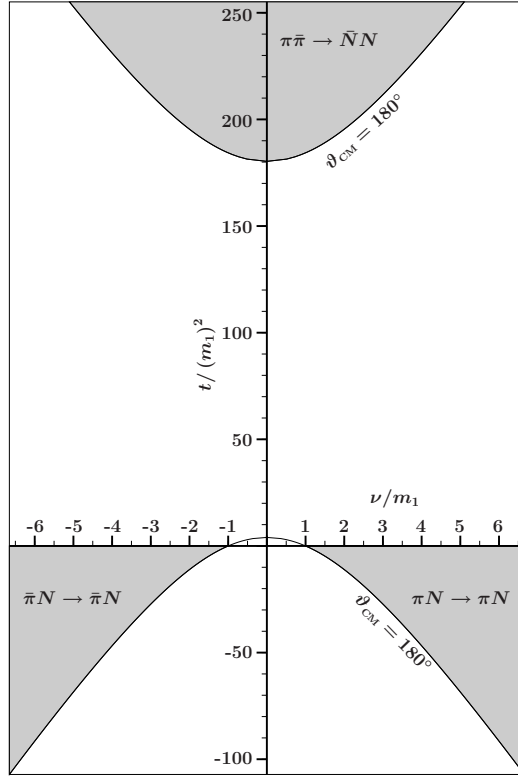


Figure 6.7: The physically allowed regions (shaded areas) in the (ν, t) plane for the three channels related to elastic πN scattering ($m_1 = m_\pi = 0.14$ GeV, $m_2 = m_N = 0.94$ GeV). The shaded areas, which are understood to extend to infinity, represent respectively the physically allowed region for πN (lower right), for $\bar{\pi}N$ (lower left) and for $\pi\bar{\pi} \rightarrow \bar{N}N$ (top). The solid lines result from formulas (6.34) and (6.50) for constant ϑ_{CM} .

6.4.2 The transition-matrix elements

In the t channel, where the scattering process is given by $\pi\bar{\pi} \rightarrow \bar{N}N$, we have to consider total isospin 0 and 1. The corresponding transition-matrix elements are denoted $T^{(+)}$ for isospin 0 and $T^{(-)}$ for isospin 1. From the crossing relations one has

$$T^{(+)} = \frac{1}{3} \left(T^{(\frac{1}{2})} + 2T^{(\frac{3}{2})} \right) \quad \text{and} \quad T^{(-)} = \frac{1}{3} \left(T^{(\frac{1}{2})} - T^{(\frac{3}{2})} \right) . \quad (6.51)$$

The reverse relations are

$$T^{(\frac{1}{2})} = T^{(+)} + 2T^{(-)} \quad \text{and} \quad T^{(\frac{3}{2})} = T^{(+)} - T^{(-)} . \quad (6.52)$$

Using the relations (6.52), we may express the processes (6.1) in $T^{(+)}$ and $T^{(-)}$. This is shown in table (6.2).

process	transition-matrix element
$\langle \pi^+ p T \pi^+ p \rangle = \langle \pi^- n T \pi^- n \rangle$	$T^{(+)} - T^{(-)}$
$\langle \pi^+ n T \pi^+ n \rangle = \langle \pi^0 n T \pi^0 n \rangle$	$T^{(+)} + T^{(-)}$
$\langle \pi^- p T \pi^- p \rangle = \langle \pi^0 p T \pi^0 p \rangle$	$T^{(+)}$
$\langle \pi^0 n T \pi^- p \rangle = \langle \pi^0 p T \pi^+ n \rangle$	$-\sqrt{2}T^{(-)}$

Table 6.2: πN processes

The process(es) we have under study is given by

$$\pi(q) + N(p) \longrightarrow \pi(q') + N(p') . \quad (6.53)$$

Hence, in terms of the momenta which are defined in formula (6.3), we define here

$$q = p_1 \quad , \quad q' = p_3 \quad , \quad p = p_2 \quad \text{and} \quad p' = p_4 . \quad (6.54)$$

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