5 Scattering Theory

"It is impossible to overemphasize the importance of this subject" (J.J. Sakurai)

5.1 The Lippmann-Schwinger equation

Let us begin with a time-independent formulation of a scattering process off a potential V:

$$H = H_0 + V \tag{5.1}$$

where

$$H_0 = \frac{\vec{p}^2}{2m} \tag{5.2}$$

is the free Hamiltonian of the scattering particle. In the absence of a scatterer, V would be zero, and the free particle state $|\vec{p}\rangle$ would be an eigenstate. If the scattering process is <u>elastic</u>, there is no change in energy and we are interested in the solution to the full Schrödinger equation with the same energy eigenvalue. More specifically, let $|\phi\rangle$ be an energy eigenvalue of H_0:

$$H_0 |\phi\rangle = E |\phi\rangle \tag{5.3}$$

(we change from $|\vec{p}\rangle$ to $|\phi\rangle$, since we will later be interested in free spherical instead of plane waves.) We wish to solve the full Schrödinger equation

$$(H_0 + V) |\psi\rangle = E |\psi\rangle \tag{5.4}$$

with E in (5.3) and (5.4) being the <u>same</u> energy eigenvalue, and

$$|\psi\rangle \to |\phi\rangle \quad \text{for } V \to 0. \tag{5.5}$$

An <u>attempt</u> to solving (5.4) may be

$$|\psi\rangle \overset{?}{=} \frac{1}{E-H_0} V|\psi\rangle + |\phi\rangle \tag{5.6}$$

In fact $|\psi\rangle \overset{(5.6)}{\rightarrow} |\phi\rangle$ for $V \to 0$ and for $H_0 \neq E$ (in an eigenvalue sense), (5.6) implies

$$V|\psi\rangle \overset{?}{=} (E-H_0)|\psi\rangle \tag{5.7}$$

such that upon insertion into (5.4), we get

$$\cancel{H_0|\psi\rangle} + (E-\cancel{H_0)|\psi\rangle} \; , = E|\psi\rangle . \quad \checkmark \tag{5.8}$$

Here, however, we had to use that $H_0 \neq E$ which is at least violated in the asymptotic limit $V \to 0$. As a purely technical solution at this point, we make the energy eigenvalue slightly complex:

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E-H_0 \pm i\varepsilon} V|\psi^{(\pm)}\rangle \tag{5.9}$$

This is the Lippmann - Schwinger equation

The meaning of the $\pm i\varepsilon$ prescription will be discussed below. Let us project this general equation onto position space

$$\langle \vec{x} | \psi^{(\pm)} \rangle = \langle \vec{x} | \phi \rangle + \int d^3x' \langle \vec{x} | \frac{1}{E-H_0 \pm i\varepsilon} | \vec{x}' \rangle \langle \vec{x}' | V | \psi^{(\pm)} \rangle . \qquad (5.10)$$

This is an integral equation, as the desired wave function on the LHS also appears under the integral. If $|\phi\rangle$ is a plane-wave state with momentum $\vec{p}$; $|\phi\rangle = |\vec{p}\rangle$, the first term in (5.10) is

$$\langle \vec{x} | \phi \rangle = \frac{e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}}{(2\pi\hbar)^{3/2}} . \qquad (5.11)$$

The kernel of (5.10) is given by the Green's function

$$G_\pm(\vec{x},\vec{x}') = \frac{\hbar^2}{2m} \langle \vec{x} | \frac{1}{E-H_0 \pm i\varepsilon} | \vec{x}' \rangle \qquad (5.12)$$

Inserting twice a complete momentum basis, we get

$$G_\pm(\vec{x},\vec{x}') = \frac{\hbar^2}{2m}\int d^3p' \int d^3p'' \underbrace{\langle \vec{x}|\vec{p}'\rangle}_{=\frac{e^{i\vec{p}'\cdot\vec{x}/\hbar}}{(2\pi\hbar)^{3/2}}} \underbrace{\langle \vec{p}'| \frac{1}{E-\frac{\vec{p}^{\,2}}{2m}\pm i\varepsilon}|\vec{p}''\rangle}_{=\frac{\delta^{(3)}(\vec{p}'-\vec{p}'')}{E-\frac{\vec{p}'^2}{2m}\pm i\varepsilon}} \underbrace{\langle \vec{p}''|\vec{x}'\rangle}_{\frac{e^{-i\vec{p}''\cdot\vec{x}'/\hbar}}{(2\pi\hbar)^{3/2}}}$$

$$= \frac{\hbar^2}{2m}\int \frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{i\vec{p}'\cdot(\vec{x}-\vec{x}')/\hbar}}{E-(\vec{p}'^2/2m)\pm i\varepsilon} . \qquad (5.13)$$

Writing $E = \frac{\hbar^2 k^2}{2m}$ and setting $\vec{p}' = \hbar\vec{q}$, this yields

$$G_\pm(\vec{x},\vec{x}') = \int\frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{i\vec{q}(\vec{x}-\vec{x}')}}{k^2-\vec{q}^{\,2}\pm i\varepsilon}$$

$$= \frac{1}{(2\pi)^3}\underbrace{\int_0^\infty dq\, q^2}_{\frac{1}{2}\int_{-\infty}^{\infty}dq} \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_{-1}^{1} d(\cos\theta) \frac{e^{i|\vec{q}||\vec{x}-\vec{x}'|\cos\theta}}{k^2-q^2\pm i\varepsilon}$$

$$= -\frac{1}{8\pi^2}\frac{1}{i|\vec{x}-\vec{x}'|}\int_{-\infty}^{\infty} dq\, q \, \frac{\left(e^{iq|\vec{x}-\vec{x}'|}-e^{-iq|\vec{x}-\vec{x}'|}\right)}{q^2-k^2\mp i\varepsilon}$$

(5.14)

The integrand has poles in the complex q-plane

$$q = \pm k \sqrt{1 \pm \left(\frac{i\varepsilon}{k^2}\right)} \simeq \pm k \pm i\,\varepsilon' \qquad (5.15)$$

Depending on the $\pm$ choice for the $i\varepsilon$ prescription, we can close the contour in the upper or lower complex q plane at infinity and use the method of residues to evaluate (5.14):

$$G_\pm(\vec{x},\vec{x}\,') = -\frac{1}{4\pi}\,\frac{e^{\pm ik|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|} \,. \qquad (5.16)$$

This is, in fact, the Green's function of the Helmholtz equation

$$\left(\vec{\nabla}^2 + k^2\right) G_\pm(\vec{x},\vec{x}\,') = \delta^{(3)}(\vec{x}-\vec{x}\,') \qquad (5.17)$$

known from classical electrodynamics.

To summarize, the Lippmann-Schwinger

equation now yields

$$\langle \vec{x} \,|\, \psi^{(\pm)} \rangle = \langle \vec{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \, \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|} \langle \vec{x}' | V | \psi^{(\pm)} \rangle \tag{5.18}$$

with the first term representing the incident wave and the second term denoting the effect of the scattering process. This second term is an example for Huygens principle, where the result of the scattering is a superposition of outgoing (+) or incoming (−) spherical waves originating from the scattering potential. As most physical systems correspond to the case where we observe outgoing plane/spherical waves (instead of preparing the system with incoming spherical waves), the (+) solution is more relevant for us.

Let us specialize to the case where the potential is said to be local, i.e.

$$\langle \vec{x}' | V | \vec{x}'' \rangle = V(\vec{x}')\, \delta^{(3)}(\vec{x}' - \vec{x}'') \tag{5.19}$$

$$\Rightarrow \langle \vec{x}' | V | \psi^{(\pm)} \rangle = V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle \tag{5.20}$$

such that (5.18) yields

$$\langle \vec{x} | \psi^{(\pm)} \rangle = \langle \vec{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \, \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi |\vec{x}-\vec{x}'|} \, V(\vec{x}') \langle \vec{x}' | \psi^{(\pm)} \rangle \tag{5.21}$$

Let us adapt this equation to a typical physics situation, where the scattering potential is rather well localized (say a nucleus of an atom). In such a case, the main contribution to the $\vec{x}'$ integral arises from a finite region in position space which we may consider as bounded. Furthermore, the detector at $\vec{x}$ is typically put far away from this scattering region such that

$$|\vec{x}| \gg |\vec{x}'| \tag{5.22}$$

if the localized potential region sits near the origin of our coordinate system.

Introducing

$$\begin{aligned} r &= |\vec{x}| \\ r' &= |\vec{x}'| \\ \alpha &= \sphericalangle(\vec{x}, \vec{x}'), \end{aligned} \tag{5.23}$$

we have for $r \gg r'$:

$$\begin{aligned} |\vec{x} - \vec{x}'| &= \sqrt{r^2 - 2rr'\cos\alpha + r'^2} \\ &\simeq r\left(1 + \frac{r'}{r}\cos\alpha + \mathcal{O}\left(\frac{r'^2}{r^2}\right)\right) \\ &= r - \hat{e}_r \cdot \vec{x}'. \end{aligned} \tag{5.24}$$

Let us also define the outgoing wave vector as

$$\vec{k}' = k \cdot \hat{e}_r \tag{5.25}$$

Its modulus is fixed to k for an elastic scattering process and we may be observing the outgoing wave along the direction $\hat{e}_r$. The spherical wave factor in (5.21) then reduces to

$$e^{\pm ik|\vec{x}-\vec{x}'|} \simeq e^{\pm ikr \mp i\vec{k}'\cdot\vec{x}'} \tag{5.26}$$

for large r. Similarly, we replace $\frac{1}{|\vec{x}-\vec{x}'|}$ just by $\frac{1}{r}$ (higher order could, of course, be included as well). It is often a standard convention to use $|\phi\rangle = |\vec{k}\rangle$ states (instead of $|\vec{p}=\hbar\vec{k}\rangle$) in order to get rid of the $\hbar$ factors, i.e.

$$\langle\vec{x}|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}} . \tag{5.27}$$

Then (5.21) becomes

$$\langle\vec{x}|\psi^{(+)}\rangle \xrightarrow{r\to\infty} \langle\vec{x}|\vec{k}\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' \, \frac{e^{ikr}}{r} e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}')$$

$$V(\vec{x}')\langle\vec{x}'|\psi^{(+)}\rangle$$

$$= \frac{1}{(2\pi)^{3/2}}\left(e^{i\vec{k}\cdot\vec{x}} + \frac{e^{ikr}}{r} f(\vec{k}',\vec{k})\right) \tag{5.28}$$

where we confined ourselves to the $(+i\varepsilon)$ prescription for the outgoing-wave boundary condition.

Eq. (5.28) thus describes an ~~outgoing~~ incoming plane-wave in propagation direction $\vec{k}$ plus an outgoing spherical wave with amplitude $f(\vec{k}',\vec{k})$ given by

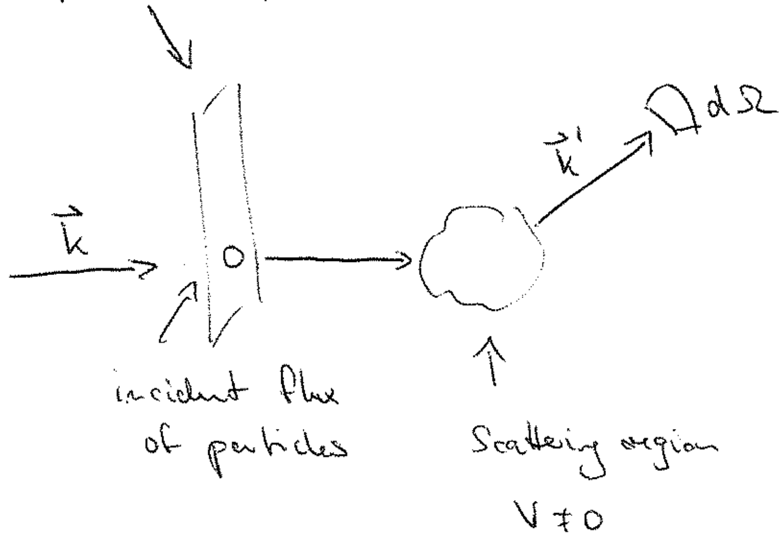
$$\underline{\underline{f(\vec{k}',\vec{k})}} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\int d^3x \underbrace{\frac{e^{-i\vec{k}'\cdot\vec{x}'}}{(2\pi)^{3/2}}}_{=\langle\vec{k}'|\vec{x}'\rangle} V(\vec{x}')\langle\vec{x}'|\psi^{(+)}\rangle$$

$$(5.29)$$

$$= \underline{\underline{-\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\langle\vec{k}'|V|\psi^{(+)}\rangle}}$$

This <u>scattering</u> amplitude is a measure for the probability of an incoming particle to be scattered into the $\vec{k}'$ direction by a potential V.

To be more precise, let us define the differential cross section $\frac{d\sigma}{d\Omega}$ as the number of particles going into a small area $d\sigma$ corresponding to a differential solid-angle element $d\Omega$, normalized to the number of incident particles per unit area per unit time (crossing a plane perpendicular to the incident direction)



$$\frac{d\sigma}{d\Omega}\, d\Omega = \frac{\text{number of particles scattered into } d\Omega \text{ per unit time}}{\text{number of incident particles per unit area per unit time}}$$

$$= \frac{r^2 d\Omega \; |\vec{j}_{scatt}|}{|\vec{j}_{incid}|} \qquad (5.30)$$

Where $\vec{j}_{scatt/incid}$ are the Schrödinger currents arising from the second / first term of (5.28), respectively.

We can easily read off that

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}',\vec{k})|^2 \qquad (5.34)$$

yields the differential cross section.

(NB: The time-independent derivation presented here also applies to a fully time-dependent process of, say, a scattering of a finite wave packet off a potential, as long as the spatial extent of the wave packet is much larger as the range of the potential V.)

5.2 The Born approximation

Expressions (5.28) & (5.29) still are complicated, since the scattering amplitude still contains the unknown ket $|\psi^{(+)}\rangle$, i.e., these are still integral equations. The Born approximation ($\simeq$ 1st order perturbation theory) consists of replacing $|\psi^{(+)}\rangle$ by $|\phi\rangle$, i.e., replacing the full ket by the incoming ket $|\phi\rangle$ which is fully known:

$$\langle \vec{x} | \psi^{(+)} \rangle \to \langle \vec{x}' | \varphi \rangle = \frac{e^{i\vec{k}\cdot\vec{x}'}}{(2\pi)^{3/2}} \tag{5.32}$$

on the RHS. The first-order Born amplitude thus is

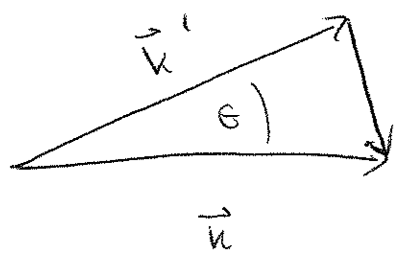
$$f^{(1)}(\vec{k}', \vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' \, e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'} \, V(\vec{x}'), \tag{5.33}$$

which is nothing but the Fourier transform of the potential (up to prefactors).

As a specific example, let us consider spherically symmetric potentials $V(r')$.

Let us specialize to the case of a spherically symmetric potential. Then $f^{(1)}(\vec{k}', \vec{k})$ is only a function of $|\vec{k}-\vec{k}'|$, as no direction $\vec{x}'$ in the integral is preferred. Also, as $|\vec{k}'| = |\vec{k}| = k$ due to energy conservation, let us write

$$|\underbrace{\vec{k}-\vec{k}'}_{\vec{q}}| \equiv q = 2k \sin\frac{\theta}{2} \tag{5.34}$$



Performing the angular integration, we get

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2} 2\pi \int_{-1}^{1} d(\cos\vartheta) \int_0^\infty dr\, r^2 \, e^{iqr\cos\vartheta} V(r)$$

$$= -\frac{1}{2}\frac{2m}{\hbar^2}\frac{1}{iq}\int_0^\infty \frac{dr}{r} r^2 V(r)\left(e^{iqr} - e^{-iqr}\right)$$

$$= -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty dr\, r V(r) \sin qr \,. \qquad (5.35)$$

Let us now consider the example of a Yukawa potential

$$V(r) = V_0 \frac{e^{-\mu r}}{\mu r}\,, \qquad (5.36)$$

where V_0 is a constant and $\frac{1}{\mu}$ can be interpreted as the range of the potential. In this case, the integral in (5.35) gives

$$f^{(1)}(\theta) = -\left(\frac{2mV_0}{\mu\hbar^2}\right)\frac{1}{q^2+\mu^2} \qquad (5.37)$$

As $$q^2 = 4k^2 \sin^2\frac{\theta}{2} = 2k^2(1-\cos\theta) \qquad (5.38)$$

The differential cross section for scattering off a Yukawa potential is given by

$$\left(\frac{d\sigma}{d\Omega}\right) \simeq \left(\frac{2mV_0}{\mu\hbar^2}\right)^2 \frac{1}{\left[2k^2(1-\cos\theta)+\mu^2\right]^2} \qquad (5.39)$$

In the somewhat delicate limit $\mu \Rightarrow 0$ (where the potential becomes long-range such that some of the assumptions leading to (5.39) are actually violated), it is interesting to see that $V(r)$ does not only approach the Coulomb potential if we keep $\frac{V_0}{\mu}$ fixed, e.g.

$$\frac{V_0}{r} = \frac{ZZ'e^2}{r}, \qquad (5.40)$$

but also the first-order Born differential cross section becomes

$$\left(\frac{d\sigma}{d\Omega}\right) \simeq \left(\frac{2m^2}{\hbar^2}\right) (ZZ'e^2)^2 \frac{1}{16\,k^4 \sin^4\left(\frac{\theta}{2}\right)} \qquad (5.41)$$

Or using $E_{kin} = \frac{(\hbar k)^2}{2m} = \frac{|\vec{p}|^2}{2m}$, this reduces to

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{1}{16}\left(\frac{ZZ'e^2}{E_{kin}}\right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)} \tag{5.42}$$

which is exactly the Rutherford scattering cross section that can even be obtained by classical considerations. We will come back to this "coincidence" later.

Some general remarks about the cross-section or the scattering amplitude can be made, if the first-order Born approximation is appropriate:

1. $\frac{d\sigma}{d\Omega}$ and/or $f(\theta)$ is a function of q only, i.e., it depends on the energy $\frac{\hbar^2 k^2}{2m}$ and θ only through the combination $2k^2(1-\cos\theta)$.

2. $f(\theta)$ is always real

3. $\frac{d\sigma}{d\Omega}$ is independent of the sign of V

4. For small k (and q), (5.35) reduces to

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x\, V(r) \tag{5.43}$$

involving a volume integral independent of θ.

5. $f(\theta)$ is "small" for large q due to rapid oscillations of the integrand.

Let us finally investigate the regime of validity of the Born approximation. Roughly speaking, the Born approximation should be reasonable, if $\langle \vec{x} | \psi^{(+)} \rangle$ is not too different from $\langle \vec{x} | \phi \rangle$. With regard to (5.28), this translates into

$$\left| \frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' \, \frac{e^{ikr'}}{r'} \, V(\vec{x}') \, e^{ik \cdot \vec{x}'} \right| \ll 1 \qquad (5.44)$$

This can be studied more explicitly for the Yukawa potential. For small energies $k \ll \mu$, we replace $e^{ikr'}$ by 1 and obtain

$$\frac{2m}{\hbar^2} \frac{|V_0|}{\mu^2} \ll 1 \qquad (5.45)$$

It is instructive to compare this condition with the condition for the Yukawa potential to develop a bound state which can be shown to be

$$\frac{2m}{\hbar^2}\,\frac{|V_0|}{\mu^2} \gtrsim 2.7 \,. \tag{5.46}$$

In other words, if the potential is strong enough to develop a bound state, the Born approximation will probably be misleading.
The opposite limit $k \gg \mu$ requires a careful analysis of the $\vec{x}'$ integral at large $|\vec{x}'|$, yielding the condition

$$\frac{2m}{\hbar^2}\,\frac{|V_0|}{\mu k}\ln\left(\frac{k}{\mu}\right) \ll 1 \,. \tag{5.47}$$

This inequality is more easily satisfied if k increases. This is a rather general feature of the Born approximation: it tends to get better at higher energies.

Higher-order Born approximations

For organizing higher-order Born approximations, it is useful to introduce the transition operator T, such that

$$V|\psi^{(+)}\rangle = T|\phi\rangle . \qquad (5.48)$$

Multiplying the Lippmann-Schwinger eq. (5.9) by V, we obtain

$$T|\phi\rangle = V|\phi\rangle + V\frac{1}{E-H_0+i\varepsilon}T|\phi\rangle . \qquad (5.49)$$

As $|\phi\rangle$ may represent any plane-wave ket which altogether form a complete set of states, (5.49) also holds as an operator equation,

$$T = V + V\frac{1}{E-H_0+i\varepsilon}T \qquad (5.50)$$

In this notation, the scattering amplitude (5.29) can also be written as

$$f(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \langle \vec{k}' | T | \vec{k} \rangle . \qquad (5.51)$$

In other words, once we know the transition operator T, we also know the scattering amplitude.

The definition of T in (5.49) can be iterated,

$$T = V + V\frac{1}{E-H_0+i\varepsilon}V + V\frac{1}{E-H_0+i\varepsilon}V\frac{1}{E-H_0+i\varepsilon}V + \dots \qquad (5.52)$$

Upon insertion of (5.52) into (5.51), we obtain a corresponding expansion of $f(\vec{k}',\vec{k})$,

$$f(\vec{k}',\vec{k}) = \sum_{n=1}^{\infty} f^{(n)}(\vec{k}',\vec{k}) , \qquad (5.53)$$

where n counts the number of V operators entering the amplitude,

$$f^{(1)}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \langle \vec{k}' | V | \vec{k} \rangle$$

$$f^{(2)}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \langle \vec{k}' | V\frac{1}{E-H_0+i\varepsilon}V | \vec{k} \rangle$$

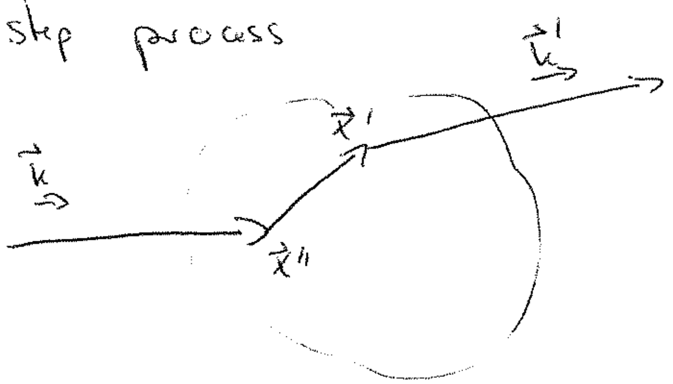
$$\vdots \qquad (5.54)$$

By inserting position space projectors, we can transform $f^{(2)}$ and higher orders into a more explicit form:

$$f^{(2)} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x' \int d^3x'' \, e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}')\left[\frac{2m}{\hbar^2} G_+(\vec{x}',\vec{x}'')\right]$$

$$\cdot \, V(\vec{x}'') \, e^{+i\vec{k}\cdot\vec{x}''} . \qquad (5.55)$$

This structure can be interpreted rather literally: the incident wave first interacts at $\vec{x}''$ with $V(\vec{x}'')$, then propagates (via $G_+(\vec{x}',\vec{x}'')$) from $\vec{x}''$ to $\vec{x}'$ where it interacts with $V(\vec{x}')$ and then is scattered into the direction $\vec{k}'$. $f^{(2)}$ hence arises as a two-step process



$f^{(3)}$ as a three-step process and so on.

The outgoing amplitude then is a sum over all possible paths and steps.

5.3 Optical theorem

The optical theorem relates the forward scattering amplitude with the total cross section

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} \, d\Omega . \qquad (5.56)$$

The precise relation is

$$\underline{\underline{\operatorname{Im} f(\theta=0) = \frac{k\sigma_{tot}}{4\pi}}} \qquad (5.57)$$

(Feenberg '32) and is straightforward to prove; we start with the exact expression (5.51)

$$f(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k}' | T | \vec{k} \rangle \qquad (5.58a)$$

which for the forward direction reduces to

$$f(\vec{k}, \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k} | T | \vec{k} \rangle \qquad (5.58b)$$

Using the definition of T in (5.48) & (5.49) (with $|\phi\rangle = |k\rangle$)

we deduce

$$\mathrm{Im}\,\langle \vec{k}\,|T|\,\vec{k}\rangle = \mathrm{Im}\,\langle \vec{k}\,|V|\,\psi^{(+)}\rangle$$

$$= \mathrm{Im}\left[\left(\langle\psi^{(+)}| - \langle\psi^{(+)}|V\frac{1}{E-H_0-i\varepsilon}\right)V|\psi^{(+)}\rangle\right] \tag{5.51}$$

hermitean conjugation

where we also used that V is hermitean.
Using the relation between pole structures, principle value integrals and the δ function,

$$\frac{1}{E-H_0-i\varepsilon} = \mathcal{P}\frac{1}{E-H_0} + i\pi\,\delta(E-H_0)\,, \tag{5.52}$$

we get

$$\mathrm{Im}\,\langle \vec{k}\,|T|\,\vec{k}\rangle = \mathrm{Im}\left(\langle\psi^{(+)}|V|\psi^{(+)}\rangle\right)$$

$$- \mathrm{Im}\left(\langle\psi^{(+)}|V\,\mathcal{P}\frac{1}{(E-H_0)}\,V|\psi^{(+)}\rangle\right)$$

$$- \mathrm{Im}\left(\langle\psi^{(+)}|\,i\pi\,\delta(E-H_0)\,|\,\psi^{(+)}\rangle\right) \tag{5.53}$$

Due to Hermiticity, the matrix elements in the first two terms are manifestly real, implying that their imaginary parts vanish

$$\Rightarrow \quad \mathrm{Im}\,\langle \vec{k}|T|\vec{k}\rangle$$

$$= -\pi \langle \psi^{(+)}| V\,\delta(E-H_0)\,V|\psi^{(+)}\rangle$$

$$= -\pi \langle \vec{k}|T^{+}\delta(E-H_0)\,T|\vec{k}\rangle$$

$$= -\pi \int d^3k' \langle \vec{k}|T^{+}|\vec{k}'\rangle\langle \vec{k}'|T|\vec{k}\rangle\, \delta\left(E-\frac{\hbar^2 k'^2}{2m}\right)$$

$d^3k' = k'^2\, dE\, \frac{dk'}{dE}\, d\Omega'$

$k' = k$ ↑ elastic scattering

$$= -\pi \int d\Omega' \frac{mk}{\hbar^2} |\langle \vec{k}'|T|\vec{k}\rangle|^2 \qquad (5.54)$$

(5.58b)

$$\Rightarrow \mathrm{Im} f(0) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\left(-\frac{\pi m k}{\hbar^2}\int d\Omega' \underbrace{|\langle \vec{k}'|T|\vec{k}\rangle|^2}_{\sim |f(\vec{k}',\vec{k})|^2}\right)$$

$$= \frac{k\sigma_{tot}}{4\pi} \qquad (5.55)$$

We will see later that the imaginary part is roughly a measure for what is missing of the incident wave in the forward direction. Due to probability conservation, this scattered piece of the incident wave has to go "somewhere".

On the other hand, the total cross section is a measure for what has been scattered "at all".

So a relation between $\mathrm{Im}\, f(0)$ and σ_{tot} appears naturally and thus is quantified by the optical theorem.

5.5 plane waves vs. spherical waves

So far, we have considered plane wave solutions as concrete representations for the eigenstates of the free propagation. For radially symmetric scatterers, the partial-wave analysis discussed below will turn out to be very useful. In this analysis, one uses the fact that angular momentum operators such as $\vec{L}^2$, L_z commute with the potential, and hence $|l\,m\rangle$ angular momentum eigenstates form a good basis together with the energy eigenkets

$$|E\,lm\rangle = |E\rangle \otimes |lm\rangle . \qquad (5.56)$$

In fact, since also $\vec{L}^2, L_z$ commute with H_0, we could equally span the incident waves by $|E\,lm\rangle$ which is called a spherical-wave basis. We adopt the normalization

$$\langle E'\,l'm' | E\,lm\rangle = \delta_{ll'}\,\delta_{mm'}\,\delta(E-E') . \qquad (5.57)$$

In order to be able to switch between the two bases, let us work out the transition amplitude $\langle \vec{k} | E\,lm\rangle$.

For this, we start with the observation that $|\vec{k} = k\hat{e}_z\rangle$ is annihilated by L_z:

$$L_z\,|k\hat{e}_z\rangle = (xp_y - yp_x)\,|k_x=0, k_y=0, k_z=k\rangle = 0 \qquad (5.58)$$

This implies that

$$m\,\langle E\,lm | k\hat{e}_z\rangle = \langle E\,lm | L_z | k\hat{e}_z\rangle = 0 \qquad (5.59)$$

meaning that

$$\langle E\, l m \,|\, k\hat{e}_z\rangle = 0 \quad \text{for } m \neq 0 . \tag{5.60}$$

This property simplifies the expansion of $|k\hat{e}_z\rangle$ in terms of spherical waves,

$$|k\hat{e}_z\rangle = \sum_{l'} \int dE' \, |E' l' m'{=}0\rangle \langle E' l' m'{=}0 \,|\, k\hat{e}_z\rangle \tag{5.61}$$

Now we construct the ket $|\vec{k}\rangle$ out of $|k\hat{e}_z\rangle$ by a suitable rotation,

$$|\vec{k}\rangle = \Gamma(R)\, |k\hat{e}_z\rangle \tag{5.62}$$

with $R \in SO(3)$, the rotation group in 3-space. R is parameterized in this case by Θ and Φ (polar and azimuthal angles); the third Euler angle is not needed here. Projection onto the spherical-wave basis gives

$$\langle E\, l m \,|\, \vec{k}\rangle \overset{(5.62)}{\underset{(5.61)}{=}} \sum_{l'} \int dE' \, \langle E\, l m \,|\, \Gamma(R) \,|\, E' l' m'{=}0\rangle \cdot \langle E' l' m'{=}0 \,|\, k\hat{e}_z\rangle$$

$$\overset{(3.52)}{=} \sum_{\ell'} \int dE' \, D^{(\ell')}_{m0}(\theta,\varphi) \, \delta_{\ell\ell'} \, \delta(E-E') \, \langle E' \ell' m'=0 | k\hat{e}_z \rangle$$

$$= D^{(\ell)}_{m0}(\theta,\varphi) \, \langle E \, \ell \, m=0 \, | \, k\hat{e}_z \rangle \qquad (5.63)$$

Here, we need $D^{(\ell)}_{m0}(\theta,\varphi)$ which rotates the $\hat{e}_z$ vector into the direction $\hat{n} = n(\theta,\varphi)$,

$$|\hat{n}\rangle = \Gamma\,(R(\theta,\varphi))\,|\hat{e}_z\rangle \qquad (5.64)$$

$$\Rightarrow \quad \langle \ell m' | \hat{n} \rangle = \sum_m D^{(\ell)}_{m'm}(\theta,\varphi) \, \langle \ell m | \hat{e}_z \rangle . \qquad (5.65)$$

As

$$\langle \ell m' | \hat{n} \rangle = Y^*_{\ell m}(\theta,\varphi) \qquad (5.66)$$

defines the spherical harmonics (or its complex conjugate, we find

same argument as above

$$\langle \ell m | \hat{e}_z \rangle = Y^*_{\ell m}(\theta=0, \varphi \text{ arb.}) \, \delta_{m0}$$

$$= \sqrt{\frac{(2\ell+1)}{4\pi}} \, P_\ell(\cos\theta)\Big|_{\theta=0} \, \delta_{m0}$$

$$= \sqrt{\frac{(2\ell+1)}{4\pi}} \, \delta_{m0} . \qquad (5.67)$$

As a consequence

$$D^{l}_{m0}(\theta,\varphi) = \sqrt{\frac{4\pi}{(2l+1)}}\; Y^{*}_{lm}(\theta,\varphi) \quad (5.68)$$

Returning back to (5.63), we note that

$\langle E\, l\, m=0 \mid k\hat{e}_z \rangle$ cannot depend on θ or φ,

but only on E and l, so that (5.63)

can be written as

$$\langle \vec{k} \mid E\, l\, m \rangle = g_{lE}(k)\; Y_{lm}(\hat{k}) \qquad \hat{k} = \hat{k}(\theta,\varphi) \quad (5.69)$$

where we have defined

$$\langle E\, l\, m=0 \mid k\hat{e}_z \rangle = \sqrt{\frac{2l+1}{4\pi}}\; g^{*}_{lE}(k) \,. \quad (5.70)$$

$g_{lE}(k)$ can straightforwardly be determined from

$$(H_0 - E)\,|\, E\, l\, m \rangle = 0$$

and

$$\langle \vec{k} \mid H_0 - E) = \left(\frac{\hbar^2 k^2}{2m} - E\right) \langle \vec{k} | \quad (5.71)$$

$$\Rightarrow \quad \left(\frac{\hbar^2 k^2}{2m} - E\right) \langle \vec{k} \mid E\, l\, m \rangle = 0$$

Such that $\langle \vec{k} | E\, l m \rangle$ can only be nonvanishing if $E = \hbar^2 k^2/2m$, suggesting

$$g_{lE}(k) = N\, \delta\left(\frac{\hbar^2 k^2}{2m} - E \right) \tag{5.72}$$

The normalization N can be determined from

$$\delta(E-E')\, \delta_{ll'}\, \delta_{mm'} = \langle E' l' m' | E\, l m \rangle$$

$$= \int d^3k\, \langle E' l' m' | \vec{k} \rangle \langle \vec{k} | E\, l m \rangle$$

$$\overset{\text{exercise}}{\Rightarrow} \quad N = \frac{\hbar}{\sqrt{mk}} \qquad \text{(up to a phase)}$$

$$\Rightarrow \quad \underline{\underline{g_{lE}(k)}} = \sqrt{\frac{4\pi}{2l+1}}\, \langle k\hat{e}_z | E\, l m \rangle$$

$$= \underline{\underline{\frac{\hbar}{\sqrt{mk}}\, \delta\left(\frac{\hbar^2 k^2}{2m} - E \right)}} \tag{5.73}$$

Such that

$$\langle \vec{k} | E\, l m \rangle = \frac{\hbar}{\sqrt{mk}}\, \delta\left(\frac{\hbar^2 k^2}{2m} - E \right) Y_{lm}(\hat{k}) \tag{5.74}$$

This allows us to write a free plane-wave as a superposition of free spherical waves with all possible angular momentum quantum numbers

$$|\vec{k}\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |E l m\rangle \Big|_{E=\frac{\hbar^2 k^2}{2m}} \frac{\hbar}{\sqrt{mk}} Y_{lm}^{*}(\hat{k}) \tag{5.75}$$

Similarly the transition amplitude can be studied in position space. Let us just mention the result here:

$$\langle \vec{x} | E l m\rangle = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}} \, j_l(kr) \, Y_{lm}(\hat{r}), \tag{5.76}$$

where we have used the spherical Bessel function

$$j_l(kr) = \frac{1}{2i^l} \int_{-1}^{1} d(\cos\theta) \, e^{ikr\cos\theta} \, P_l(\cos\theta) \tag{5.77}$$

The transition from (5.74) to (5.76) can be shown by using the decomposition of a plane wave

$$\frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}} = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) i^l j_l(kr) P_l(\hat{k}\cdot\hat{r}) \tag{5.78}$$

and the addition theorem

$$\sum_m Y_{lm}(\hat{r})\, Y^*_{lm}(\hat{k}) = \frac{2l+1}{4\pi}\, P_l(\hat{k}\cdot\hat{r}) \tag{5.79}$$

5.6 Method of partial waves

So far, we discussed the free case $V=0$. Let us now assume that $V \neq 0$ is a spherically symmetric scattering potential which commutes with $\vec{L}^2$ and L_z. Then, also

$$[T, \vec{L}] = 0$$

holds, implying that T is a scalar operator. According to the Wigner-Eckart theorem, T is then diagonal WRT a spherical wave basis

$$\langle E\, l' m' | T | E\, l m \rangle = T_l(E)\, \delta_{ll'}\, \delta_{mm'} \tag{5.80}$$

with the diagonal elements $T_l(E)$ depending on l but not on m. This leads to simplifications for the scattering amplitude

$$f(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \langle \vec{k}'|T|\vec{k}\rangle$$

$$= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \sum_{l,l',m,m'} \iint dE\, dE'$$

$$\langle \vec{k}'|E'l'm'\rangle \langle E'l'm'|T|Elm\rangle \langle Elm|\vec{k}\rangle$$

$$= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \frac{\hbar^2}{mk} \sum_{lm} T_l(E)\Big|_{E=\frac{\hbar^2k^2}{2m}}$$

$$\cdot\, Y_{lm}(\hat{k}') Y^*_{lm}(\hat{k})$$

$$= \frac{4\pi^2}{k} \sum_{lm} T_l(E)\Big|_{E=\frac{\hbar^2k^2}{2m}} Y_{lm}(\hat{k}') Y^*_{lm}(\hat{k}) \tag{5.81}$$

Let us choose a coordinate system in which $\hat{k}$ defines the positive z-direction; then

$$Y_{lm}(\hat{k}) = \sqrt{\frac{2l+1}{4\pi}}\, \delta_{m0} \tag{5.82}$$

As only $m=0$ terms can contribute in (5.81), we need only

$$Y_{\ell m=0}(\hat{k}') = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) , \tag{5.83}$$

where θ is the angle between $\hat{k}$ and $\hat{k}'$.
It is conventional to define the partial wave amplitude as

$$f_\ell(k) = -\frac{\pi}{k} T_\ell(E) , \tag{5.84}$$

such that

$$f(\theta) = f(\vec{k}', \vec{k}) = \sum_{\ell=0}^{\infty} (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta) . \tag{5.85}$$

The physical significance of $f_\ell(k)$ becomes clear when we study $\langle x | \psi^{(+)} \rangle$ at large distances, where, see (5.28),

$$\langle \vec{x} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} \left[e^{ikz} + f(\theta) \frac{e^{ikr}}{r} \right] \tag{5.86}$$

Using (5.78) as well as the large r asymptotics of the spherical Bessel function

$$j_\ell(kr) \xrightarrow{r\to\infty} \frac{e^{i(kr - \ell\frac{\pi}{2})} - e^{-i(kr - \ell\frac{\pi}{2})}}{2ikr} , \quad i^\ell = e^{i\ell\frac{\pi}{2}} , \tag{5.87}$$

we find

$$\langle \vec{x} | \psi^{(+)} \rangle \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \left\{ \sum_l (2l+1) P_l(\cos\theta) \left(\frac{e^{ikr} - e^{-i(kr - l\pi)}}{2ikr} \right) + \sum_l (2l+1) P_l(\cos\theta) f_l(k) \frac{e^{ikr}}{r} \right\}$$

$$= \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l}{2ik} \left\{ (1 + 2ikf_l(k)) \frac{e^{ikr}}{r} - \frac{e^{-i(kr - l\pi)}}{r} \right\} \tag{5.88}$$

So, in absence of the scatterer, the incoming plane wave is written as a superposition of incoming & outgoing spherical waves. In the presence of the scatterer, only the outgoing spherical wave is modified as

$$1 \to 1 + 2ik f_l(k) \tag{5.89}$$

The incoming wave remains unaffected.

The partial wave amplitude is constraint by probability conservation, as the incoming and the outgoing probability flux must be equal. Defining

$$S_\ell(k) = 1 + 2ik f_\ell(k) \qquad (5.90)$$

this constraint implies

$$|S_\ell(k)| = 1 . \qquad (5.91)$$

This <u>unitarity relation</u> follows from probability conservation <u>and</u> rotational invariance. Only for the latter case, the partial wave probabilities do not mix and thus must satisfy the unitarity relation separately. (S_ℓ can be viewed as the ℓth diagonal element of the S matrix in partial wave decomposition).

Scattering can thus only induce a change of phase of the outgoing wave,

$$S_\ell(k) = e^{2i\delta_\ell}, \tag{5.92}$$

where δ_ℓ is the "phase shift" or "scattering phase", and the factor 2 is just a convention. This implies that f_ℓ can be parameterized by this phase, as

$$f_\ell = \frac{S_\ell - 1}{2ik} = \frac{e^{2i\delta_\ell} - 1}{2ik} \tag{5.93a}$$

$$= \frac{e^{i\delta_\ell}\sin\delta_\ell}{k} = \frac{1}{k\cot\delta_\ell - ik}, \tag{5.93b}$$

whichever is convenient. The full scattering amplitude then reads, e.g.

$$f(\theta) = \sum_{\ell=0} (2\ell+1)\left(\frac{e^{2i\delta_\ell}-1}{2ik}\right) P_\ell(\cos\theta)$$

$$= \frac{1}{k}\sum_{\ell=0} (2\ell+1)\, e^{i\delta_\ell}\sin\delta_\ell\, P_\ell(\cos\theta). \tag{5.94}$$

Let us verify the optical theorem within the partial-wave formalism,

$$\sigma_{tot} = \int |f(\theta)|^2 \, d\Omega$$

$$= \frac{1}{k^2} \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \sum_l \sum_{l'} (2l+1)(2l'+1)$$

$$\cdot \, e^{i\delta_l} \sin\delta_l \, e^{-i\delta_{l'}} \sin\delta_{l'} \, P_l P_{l'}$$

$\int_{-1}^{1} du \, P_l(u) P_{l'}(u) = \frac{2}{2l+1} \delta_{ll'}$

$$= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l \qquad (5.95)$$

On the other hand,

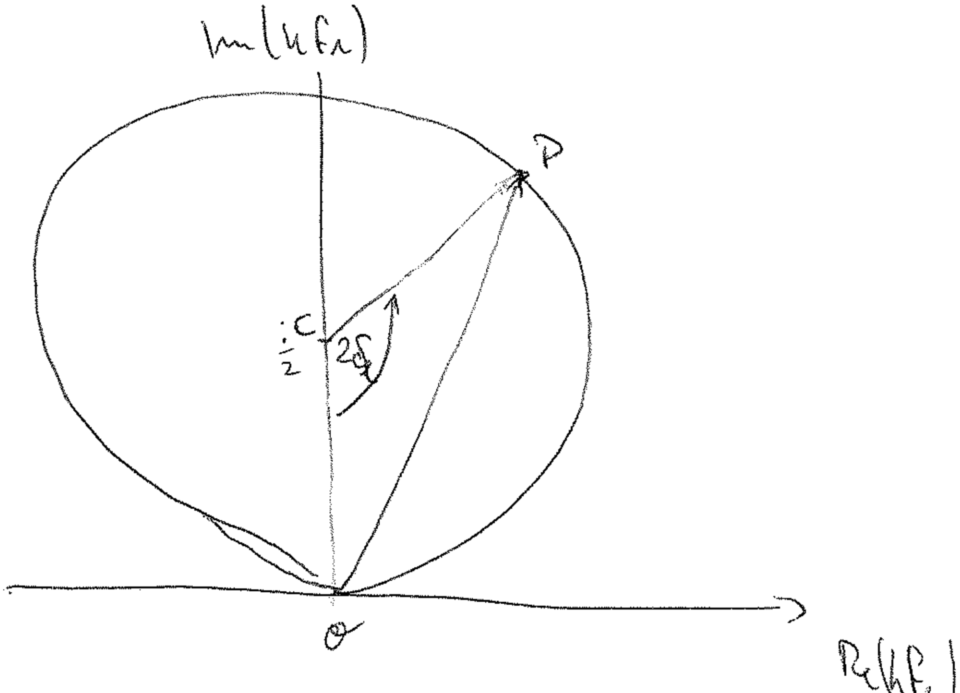
$$\mathrm{Im}\, f(\theta=0) = \sum_l \frac{(2l+1)}{k} \mathrm{Im}\left(e^{i\delta_l} \sin\delta_l\right) P_l(\cos\theta)\Big|_{\theta=0}$$

$$= \sum_l \frac{(2l+1)}{k} \sin^2\delta_l, \qquad (5.96)$$

in agreement with (5.95) up to the required factor $\frac{4\pi}{k}$.

The Phase shifts depend on l but also on the energy or on k. The unitarity relation (5.90) constrains the way how f_l and δ_l can depend on k. This can be visualized by an Argand diagram. Let us plot kf_l in a complex plane using (5.93a)

$$kf_l = \frac{i}{2} + \frac{1}{2} e^{-\left(i\frac{\pi}{2}\right) + 2i\delta_l} \qquad (5.97)$$



OP is the magnitude of kf_l. The phase shift is related to the angle in the triangle CPO. The circle on which kf_l must lie is known as the <u>unitary circle</u>.

For small δ_ℓ, kf_ℓ is near the bottom of the circle and hence f_ℓ is almost purely real,

$$f_\ell = e^{i\delta_\ell}\frac{\sin\delta_\ell}{k} \simeq \frac{(1+i\delta_\ell)\,\delta_\ell}{k} \simeq \frac{\delta_\ell}{k}\,, \tag{5.98}$$

whereas if δ_ℓ is close to $\frac{\pi}{2}$, the partial cross section becomes maximal

$$\sigma^{(\ell)}_{max} = \frac{4\pi}{k^2}(2\ell+1)\cdot \underbrace{1}_{=\,\sin^2\delta_\ell\big|_{\delta_\ell=\frac{\pi}{2}}} \tag{5.99}$$

Determination of phase shifts

Let us work out how to determine phase shifts for a potential V. Let us assume that V vanishes outside a finite "range" R, i.e. $V=0$ for $r>R$. This means that outside the wave function must be that of a free spherical wave. In (5.76), we found the position space representation

$$\langle \vec{x} | E l m \rangle \sim j_l(kr)\, Y_{lm}(\hat{r}) , \qquad (5.100)$$

or for a particular choice of koordinates, $\hat{k} \sim \hat{e}_z$

$$\psi^{(+)}(\vec{x}) \sim j_l(kr)\, P_l(\cos\theta) . \qquad (5.101)$$

As $\psi^{(+)}(\vec{x})$ is a solution of a second order differential equation, there must be another linearly independent solution. In fact, this can be shown to be of the type

$$\sim n_l(kr)\, P_l(\cos\theta) , \qquad (5.102)$$

where $n_\ell(kr)$ is the spherical Neumann function. $n_\ell(kr)$ does not occur in (5.100) and is also ruled out as a solution for the region "inside", $r \le R$, as $n_\ell(kr)$ diverges at zero argument. It thus violates the boundary conditions of the radial Schrödinger equation at $r=0$. However, it is an admissible solution for the outside region as it is regular for all $r > 0$.
Alternatively to the spherical Bessel & Neumann functions, one can use the spherical Hankel functions,

$$h_\ell^{(1)} = j_\ell + i n_\ell \quad , h_\ell^{(2)} = j_\ell - i n_\ell , \qquad (5.103)$$

which asymptotically behave as

$$h_\ell^{(1)} \xrightarrow{r\to\infty} \frac{e^{i(kr - \ell\frac{\pi}{2})}}{ikr} \quad , h_\ell^{(2)} \xrightarrow{r\to\infty} \frac{e^{-i(kr-\ell\frac{\pi}{2})}}{ikr} . \qquad (5.104)$$

The full wave function at any $r > R$ can then

be written as
$$\psi^{(+)}(\vec{x}) = \frac{1}{(2\pi)^{3/2}} \sum_\ell i^\ell (2\ell+1) A_\ell(r) P_\ell(\cos\theta), \quad (5.105)$$

where
$$A_\ell = c_\ell^{(1)} h_\ell^{(1)}(kr) + c_\ell^{(2)} h_\ell^{(2)}(kr) . \quad (5.106)$$

For $V=0$, A_ℓ has to coincide with j_ℓ everywhere. At large r, A_ℓ should approach (5.88),

$$\psi^{(+)}(\vec{x}) \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \sum_\ell (2\ell+1) P_\ell \left[\frac{e^{2i\delta_\ell} e^{ikr}}{2ikr} - \frac{e^{-i(kr-\ell\pi)}}{2ikr} \right]. \quad (5.107)$$

Comparison with (5.105 & 106) implies

$$c_\ell^{(1)} = \frac{1}{2} e^{2i\delta_\ell}, \quad c_\ell^{(2)} = \frac{1}{2}, \quad (5.108)$$

such that

$$A_\ell(r) = e^{i\delta_\ell} \left[\cos\delta_\ell \, j_\ell(kr) - \sin\delta_\ell \, n_\ell(kr) \right]. \quad (5.109)$$

It is now useful to consider the logarithmic derivative of the amplitude $A_\ell(r)$ at $r=R$, taken from the outside $r \to R^+$,

$$\beta_\ell := \left(\frac{r}{A_\ell} \frac{dA_\ell}{dr} \right)_{r=R} = kR \left[\frac{j_\ell'(kR)\cos\delta_\ell - n_\ell'(kR)\sin\delta_\ell}{j_\ell(kR)\cos\delta_\ell - n_\ell(kR)\sin\delta_\ell} \right] \tag{5.110}$$

Once, this derivative is known, the phase shift can be deduced,

$$\tan\delta_\ell = \frac{kR\, j_\ell'(kR) - \beta_\ell\, j_\ell(kR)}{kR\, n_\ell'(kR) - \beta_\ell\, n_\ell(kR)} . \tag{5.111}$$

The log-derivative of the amplitude β_ℓ can, in fact, be computed from the inside solution for $r<R$ and by continuity of the wave function.
The inside solution is determined by the radial Schrödinger equation:

$$\frac{d^2 u_\ell}{dr^2} + \left(k^2 - \frac{2m}{\hbar^2} V - \frac{\ell(\ell+1)}{r^2} \right) u_\ell = 0 \tag{5.112}$$

where

$$u_\ell = r\, A_\ell(r) \, . \tag{5.113}$$

(cf. the ideal hydrogen atom). As the amplitude has to remain finite, the boundary condition for $u_\ell(r=0)$ is

$$u_\ell(r=0) = 0 \tag{5.114}$$

This Schrödinger equation has to be integrated — numerically if necessary — up to $r=R$ starting at $r=0$. From this solution, we obtain the log-derivative at $r=R$. Because of continuity the outside solution has to be matched with the inside solution at $r=R$, implying

$$\beta_{\ell\,\text{inside}}(r=R) \equiv \beta_{\ell\,\text{outside}}(r=R) \, . \tag{5.115}$$

This fixes the phase shifts via (5.111) unambiguously and thus determines the scattering solution completely.

(NB: , (5.114) does not quantize the solutions , , (two boundary conditions would be needed for this), the solutions typically form a one-parameter family of solutions:

By (5.112), this one parameter is related to the energy (or the wave number) k.)

5.7 Low-energy scattering and bound states

At low energies, i.e. small k, the wavelength $\lambda = \frac{1}{k}$ can become comparable or even larger than the range R of the potential. Classically, we would guess that higher-l partial waves become less and less important, as the inside region is classically forbidden due to the centrifugal barrier,

$$V_{eff} = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} . \qquad (5.116)$$

Unless the potential is strong enough to accommodate $\ell \neq 0$ bound states near $k \simeq 0$, the radial wave function is largely determined by the centrifugal barrier. Hence, the j_ℓ-type of contributions are expected to dominate.

Arguments similar to the Born approximation then lead to an estimate of the phase shift:

$$\underbrace{\frac{e^{i\delta_\ell}\sin\delta_\ell}{k}}_{f_\ell(k)} = -\frac{2\mu}{\hbar^2}\int_0^\infty \underbrace{j_\ell(kr)}_{\langle k|} V(r) \underbrace{A_\ell(r)}_{|\psi^{(+)}\rangle} r^2\,dr \qquad (5.117)$$

If $A_\ell(r)$ is not too different from $j_\ell(kr)$ and $1/k$ is much larger than the range of the potential, we can use the asymptotics of $j_\ell(kr)$ for small argument,

$$j_\ell(x) = x^\ell \left(\frac{2^{-1-\ell}\sqrt{\pi}}{\Gamma(\frac{3}{2}+\ell)} + \mathcal{O}(x^2)\right), \qquad (5.118)$$

to deduce

$$\delta_\ell \sim k^{2\ell+1} \tag{5.119}$$

for small k. In other words, higher ℓ are suppressed by higher powers of (small) k. This is known as threshold behavior.

In other words, at low energies and for a finite range potential, only S wave scattering ($\ell=0$) is important.

As a specific example, we consider a rectangular well or barrier

$$V = \begin{cases} V_0 = \text{const} & \text{for } r < R \\ 0 & \text{otherwise} \end{cases} \qquad \begin{cases} V_0 > 0 \text{ repulsive} \\ V_0 < 0 \text{ attractive} \end{cases} \tag{5.120}$$

This simple example exhibits many features that are common to more complicated finite-range potentials.

The outside solution must be of the form (5.109),

$$A_{\ell=0} = e^{i\delta_0}\left[j_0(kr)\cos\delta_0 - n_0(kr)\sin\delta_0 \right]$$

(5.120)

As j_0, n_0 asymptotically behave like $\frac{\sin(kr)}{kr}$ and $\frac{\cos(kr)}{kr}$, this amplitude approaches

$$A_{\ell=0} \simeq \frac{e^{i\delta_0}\sin(kr+\delta_0)}{kr} . \qquad (5.121)$$

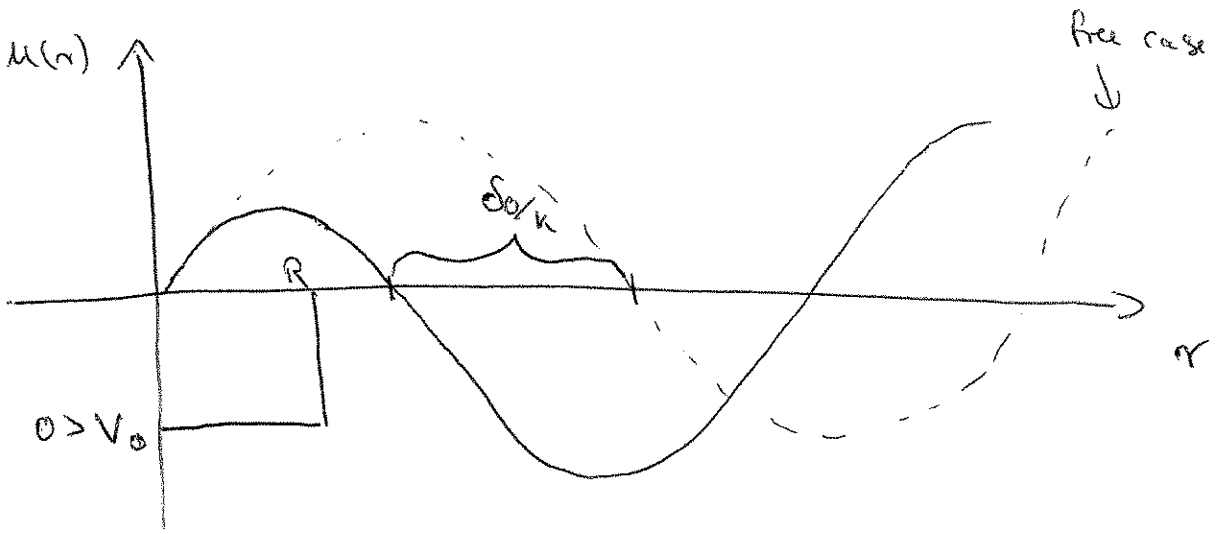
For $V_0 = \text{const.}$, the inside solution is particularly easy to get:

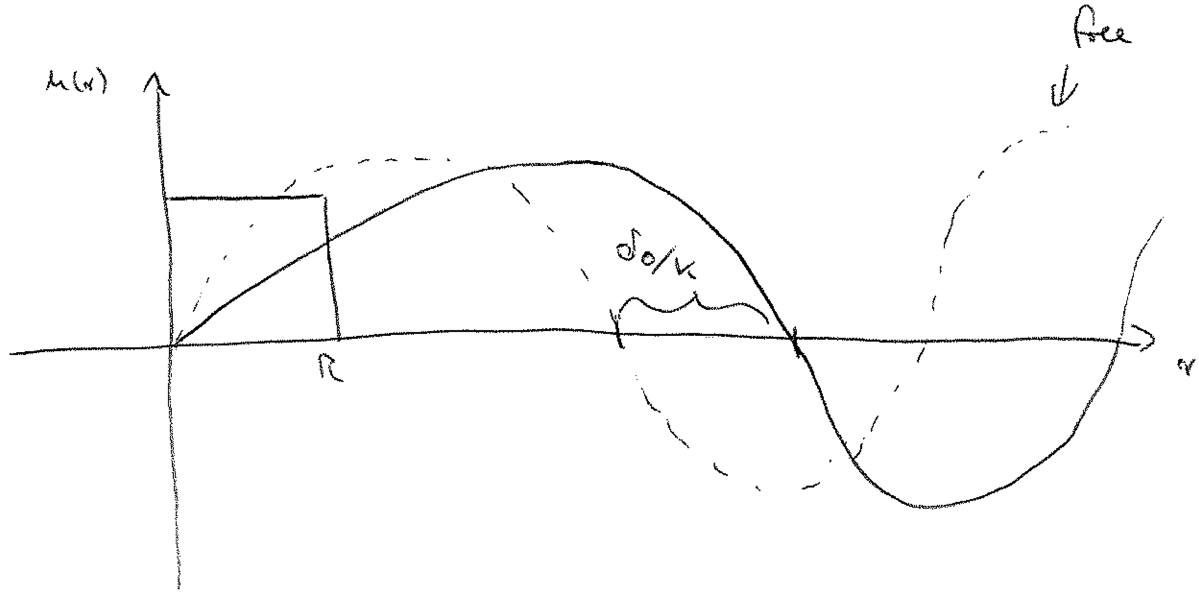
$$u_\ell = r A_{\ell=0}(r) \sim \sin k' r , \qquad (5.122)$$

where we have used the boundary condition (5.114), and k' satisfies

$$E - V_0 = \frac{\hbar^2 k'^2}{2m} . \qquad (5.123)$$

We observe that the inside wave function is still sinusoidal but with a different wavelength than the outside (free-particle) case. For attractive potentials $V_0 < 0$, the curvature of the wave function is bigger inside than outside and smaller for repulsive potentials $V_0 > 0$





This analysis also holds for $V_0 > E$

If we replace $u_\ell(r) \sim \sin kr$

by $u_\ell(r) \sim \sinh \kappa r$

with

$$\frac{\hbar^2 \kappa^2}{2m} = \left(V_0 - E\right). \qquad (5.124)$$

Let us concentrate on the attractive case. Suppose, the attraction is such that $\delta_0 = \frac{\pi}{2}$ for $kR \ll 1$. Then the S-wave cross section is maximal as $\sin^2\delta_0 = 1$

$$\Rightarrow \sigma_{max}^{(0)} = \frac{4\pi}{k^2} \qquad (5.125)$$

The ℓth scattering amplitude then is

$$f_\ell = \frac{1}{ik} \qquad (5.126)$$

such that the S matrix element

$$S_\ell = -1$$

satisfies the unitarity bound.

Many-body systems (e.g. quantum gases), where the s wave scattering is maximal in this sense have recently become very topical, as these form strongly coupled (in fact infinitely strongly coupled) quantum field theories.

Let us consider scattering at very low energies ($k \simeq 0$) in the s channel $l=0$. For $r > R$, the radial outside wave function satisfies

$$\frac{d^2 u}{dr^2} = 0 \quad . \tag{5.127}$$

The obvious solution is a straight line

$$u(r) = \text{const.} \, (r - a) \quad . \tag{5.128}$$

This can be viewed as an infinitely long wavelength limit of the usual expression for the outside wave function (5.121):

$$\lim_{k \to 0} \sin(kr + \delta_0) \sim k \left(r + \frac{\delta_0}{k} \right) \tag{5.129}$$

Similar to (5.128) with $a = -\frac{\delta_0}{k}$.

Going back to the total cross section ~~tot~~,
see, e.g., (5.99), we find

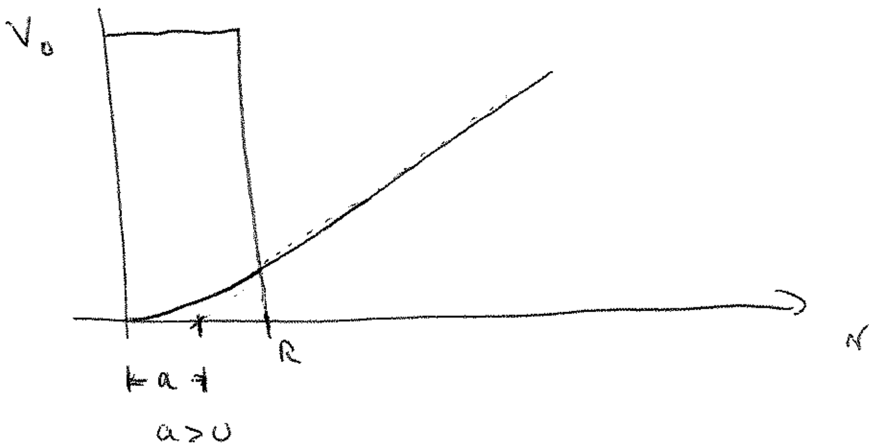
$$\sigma_{tot} \simeq \sigma_{\ell=0} = \frac{4\pi}{k^2} \sin^2\delta_0$$

$$= \frac{4\pi}{k^2} \sin^2 ak$$

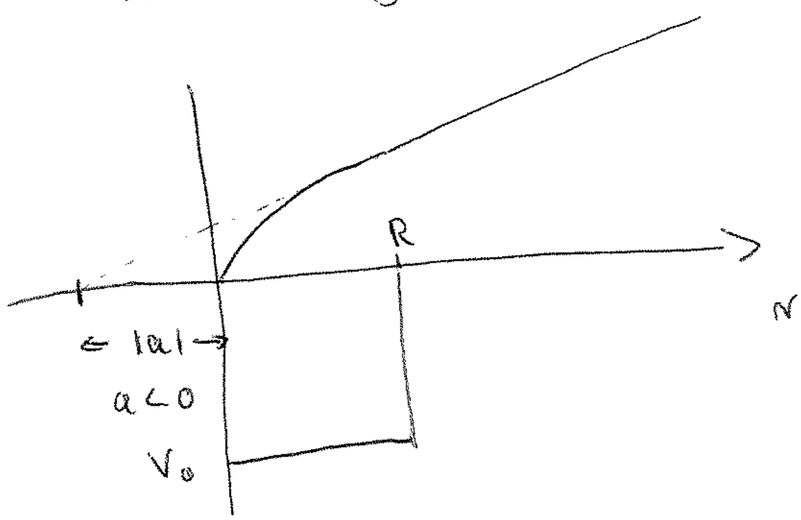
$$\xrightarrow{k\to 0} 4\pi a^2 . \qquad (5.130)$$

The quantity a has the dimension of a length. It is called the scattering length. It is interesting to note that the two length scales a and R can differ a lot. The meaning of a becomes clear from (5.128): it is the intercept of the outside wave function with the radial axis.

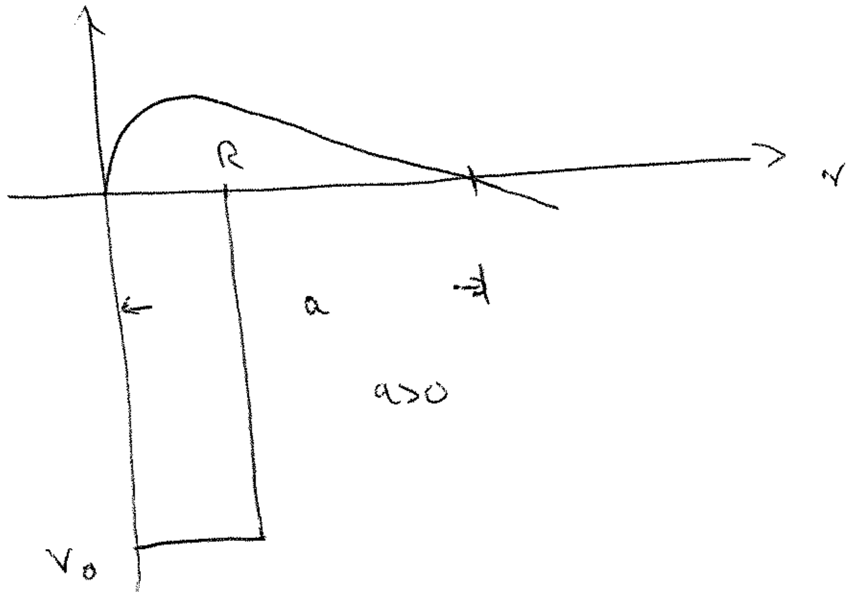
For a repulsive potential, the scattering length is positive $a>0$ and typically of order R, see figure:



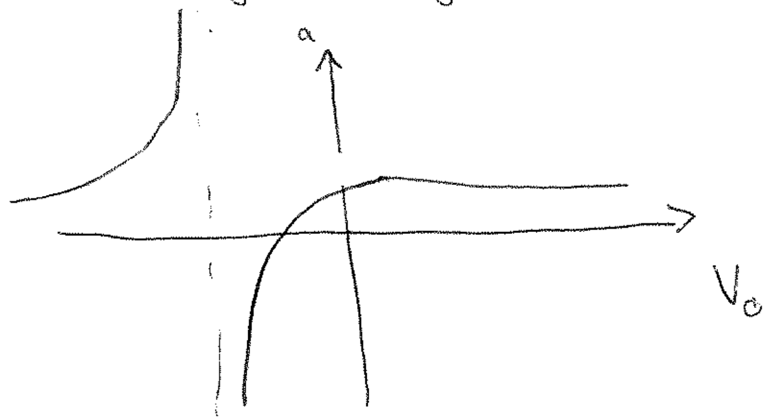
For a moderately attractive potential, the intercept is typically negative, $a<0$



If we increase the attraction, the outside wave function can again cross the r-axis on the positive side



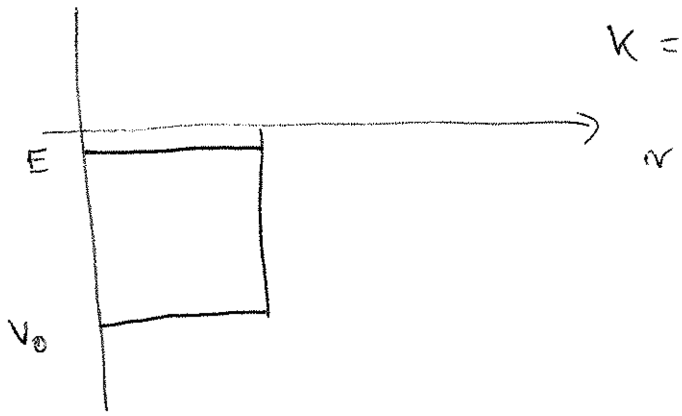
Increasing the attractive interaction between the last two figures continuously, the scattering length runs through a singularity



This singularity and the associated sign change is related to the development of a bound state. In the following, we discuss this relation on a semi-quantitative level for simplicity.

As is visible in the above pictures, the wavefunction for $r>R$ is essentially flat for large scattering length.

Similarly, the outside form of a bound state wave function $\sim e^{-\kappa r}$ is essentially flat, if the binding energy E becomes infinitesimally small



$$\kappa = \sqrt{\frac{2m}{\hbar^2}|E|}$$

The inside wave function ($r<R$) for the scattering case ($E \to 0^+$) and the bound state case ($E \to 0^-$) also become essentially identical, as k' in $\sin k'r$ (cf. (5.122), (5.123)) is determined by

$$\frac{\hbar^2 k'^2}{2m} = E - V_0 \simeq |V_0| \qquad (5.131)$$

for infinitesimal E.

As the inside wave functions are the same for the two limits, $E \to 0^\pm$, we can identify the log-derivative of the bound-state wavefunction with that of the low-energy scattering wave function:

$$-\frac{\kappa e^{-\kappa r}}{e^{-\kappa r}}\bigg|_{r=R} = \frac{1}{r-a}\bigg|_{r=R} \qquad (5.132)$$

yielding

$$\kappa \simeq \frac{1}{a} \qquad \text{for } R \ll a \qquad (5.133)$$

The binding energy then satisfies

$$\underline{\underline{E_{BE}}} = +|E| = \frac{\hbar^2\kappa^2}{2m} = \underline{\underline{\frac{\hbar^2}{2ma^2}}} \qquad (5.134)$$

relating the scattering length with the bound-state energy ! In other words, we can infer the binding energy of a loosely bound state from a measurement of the scattering length near zero kinetic energy (provided that $a \gg R$ holds).

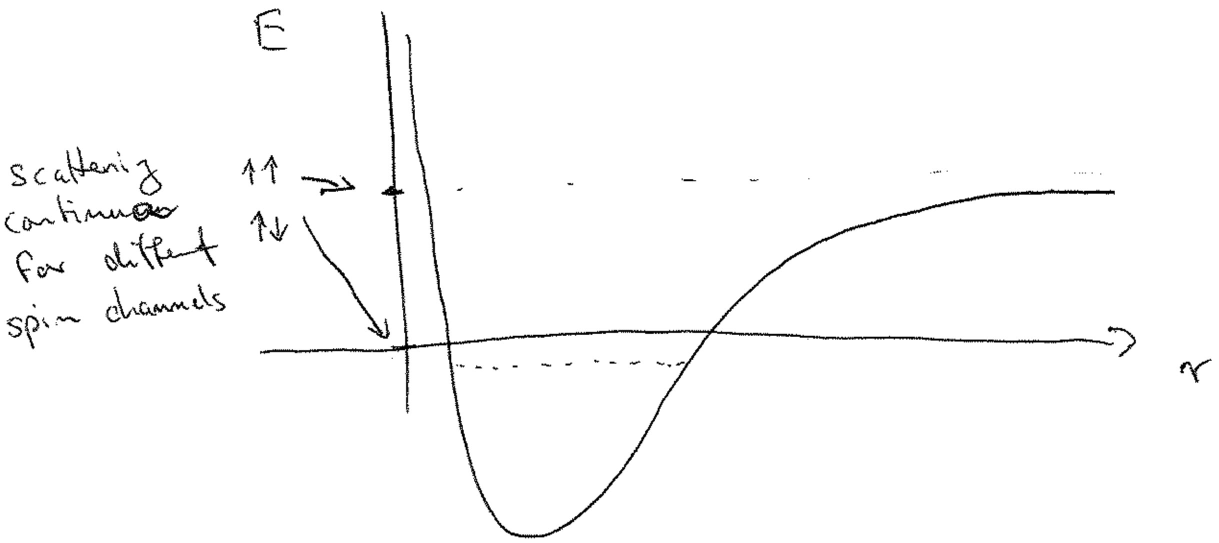
Historically, this connection was first pointed out by Wigner in an attempt to apply it to neutron-proton scattering. The bound state in this case is the deuteron with a binding energy of $E_{BE} \simeq 2.22$ MeV. Taking the measured value of the scattering length, Eq. (5.134) predicts $E_{BE} \simeq \frac{\hbar^2}{2\mu a^2} \simeq 1.4$ MeV,

μ: reduced mass $\simeq \frac{m_{n,p}}{2}$

yielding a not too satisfactory agreement. The discrepancy is also due to the fact that $a \gg R$ does not really represent a good approximation.

Recently, well-controllable systems have been identified, where the scattering length is actually tunable by hand: if atomic gases are cooled down to nano-Kelvin temperatures (by laser cooling), the kinetic energy is so low that only s-wave scattering of pairs of atoms is relevant.

In certain systems (i.e. for specific ultra-cold atom gases), the scattering continuum can energetically be in the vicinity of a bound state, which exists, for instance, in a different spin "channel":

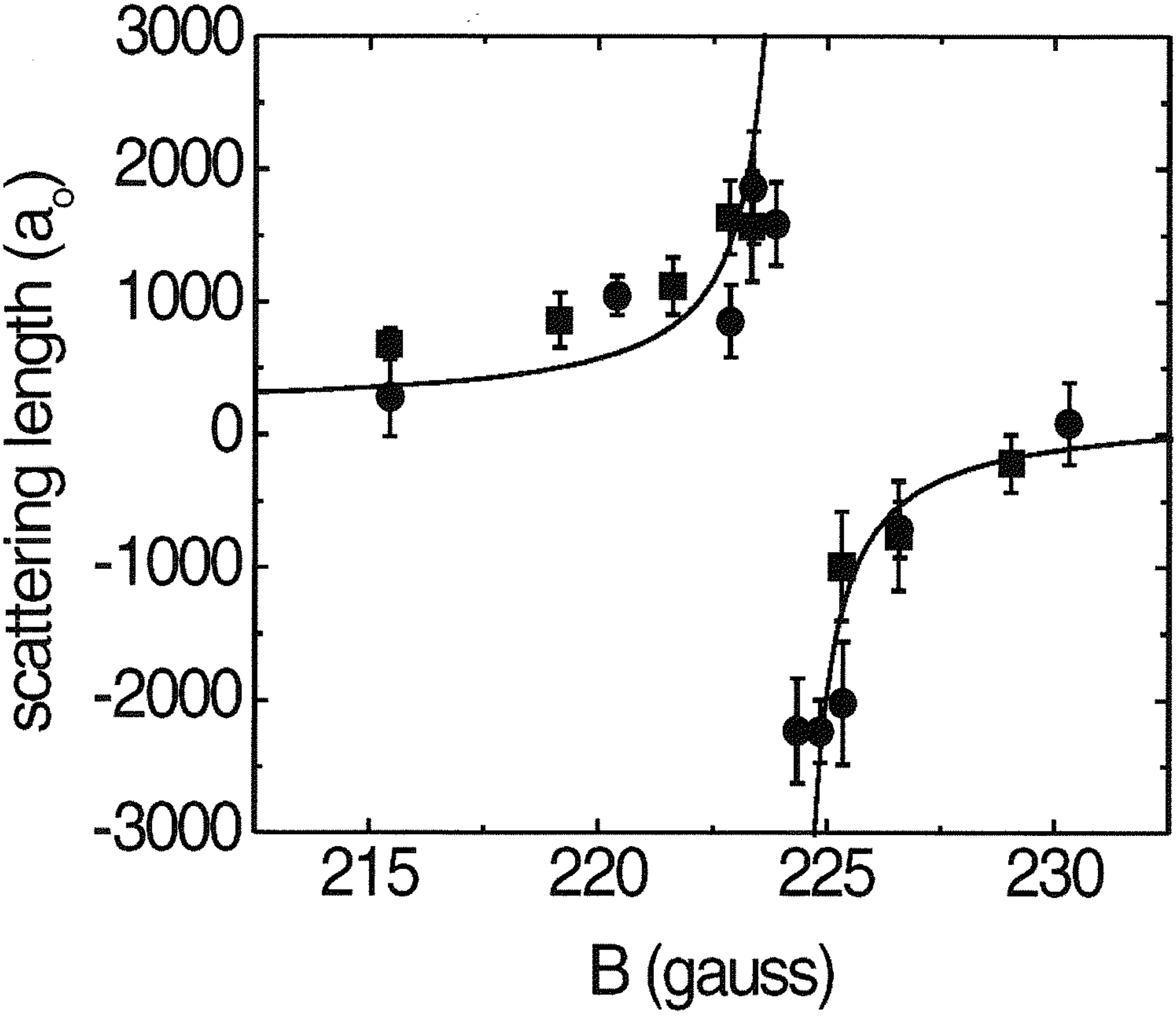


terminology: ↑↓ : open channel (accessible to freely propagating atoms)

↑↑ : closed channel (inaccessible for ultracold atoms)

In such a case, the relative height of the bound-state energy to the scattering continuum in the open channel can be tuned by an externally applied magnetic

field (Zeeman effect): varying B corresponds to varying E_{BE} and thus a by hand. The divergence of a as a function of B is called a Feshbach resonance.
In ultracold fermionic gases such as ^6Li or ^{40}K such resonances have been measured recently.
(NB: as these gases are many-body systems, they can ultimately be described by a non-relativistic quantum-field theory. In this description the coupling constant turns out to be proportional to the scattering length $\sim a$.
Feshbach resonances can thus be used to tune quantum field theories into the strong-coupling domain; this has become a very fascinating field of research both experimentally as well as theoretically. Compared to the standard realm of quantum field theory which is particle physics (where the coupling constants are determined and "fixed" by nature), being able to change the values of coupling constants



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is like changing the parameters of the universe ....)

Another relation between scattering and bound states can be inferred from taking a look at the form of the wave function solutions

$$S_{\ell=0}(k)\,\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r} \quad , \text{scattering} \qquad (5.135)$$

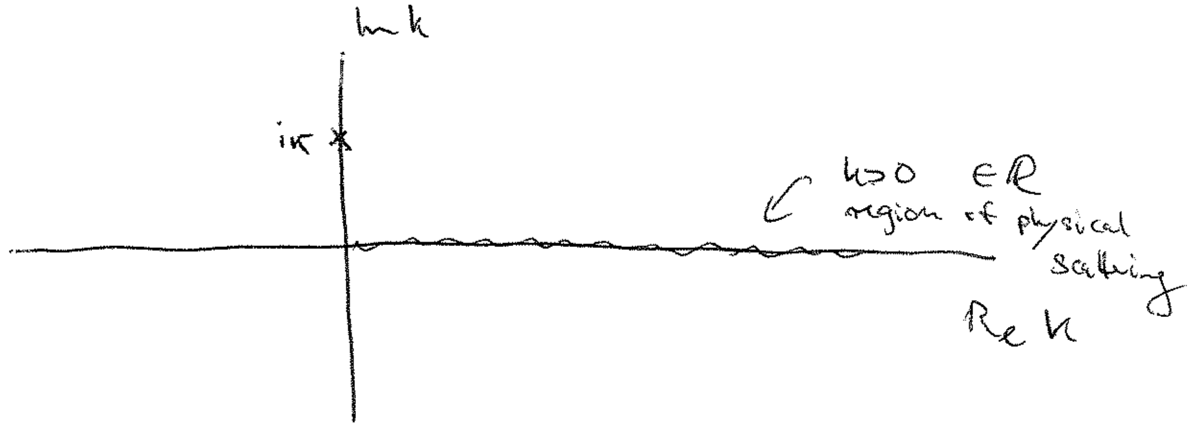
and

$$\frac{e^{-kr}}{r} \quad , \text{bound states} \qquad (5.136)$$

at large distances. We may argue that they are the same, once we identify ik with k. The important difference is that the outgoing scattering solution only exists, if there is also an incoming solution. Whereas the bound state wave function also exists without "incoming" parts in the wave packet. Concerning observables such as cross sections, only the ratio between outgoing and incoming parts are important in the scattering case $\sim S_\ell(k)$. In the bound state case, this ratio is ∞ (as there is no incoming wave).

Hence, regarding $S_{\ell=0}(k)$ as a function of $k \in \mathbb{C}$, we conclude that $S_{\ell=0}(k)$ has a pole on the imaginary axis at

$$k = i\kappa \qquad (5.137)$$



Furthermore, as $k \cot \delta_0$ approaches $-\frac{1}{a}$ for $k \to 0$ which is finite (cf. (5.129)), δ_0 must behave as

$$\delta_0 \to 0,\ \pm\pi,\ \dots \qquad (5.138)$$

such that ~~...~~ $S_{\ell=0} \to 1$ for $k \to 0$.

Hence, unitarity and the (in)existence of bound-states tightly constrains the properties of the S matrix.

With these rather qualitative remarks, we conclude our discussion of scattering theory.