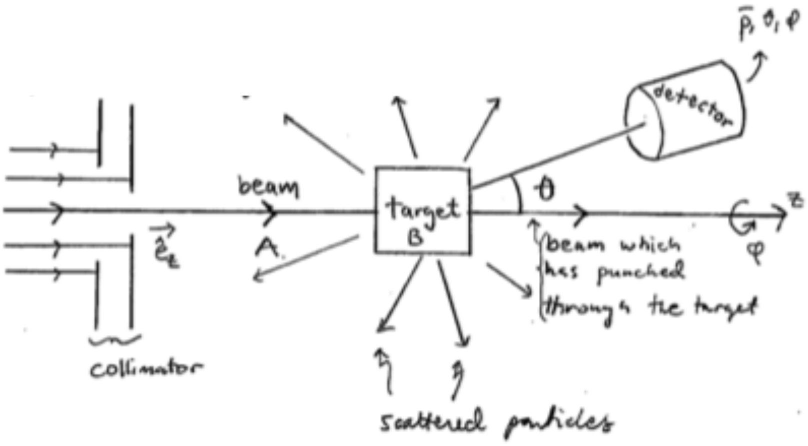
II. Scattering theory

II. 1. Basic concept: cross section

- The structure of matter is probed by doing
  - (i) **Spectroscopy**: observe transitions between the different bound states at the system (atoms, molecules, . . .)
  - (ii) **Scattering experiments**: analyze the final states and deduce the properties of target and/or beam particles (for example the structure and properties of nuclei and elementary particles, or nature of electron transport inside solids)
- A typical scattering experiment (fixed target):



$\mathbf{p}_{\text{beam}} || \hat{e}_z$

$\mathbf{p}_{\text{target}} = 0 \cong$ "fixed-target" experiment

$\mathbf{p}_{\text{target}} \neq 0 \cong$ "colliding beams" experiment

- **beam**:
  - consists of particles A (electrons, positrons, protons, neutrons, photons, phonons, . . .)
  - is nearly monoenergetic and well collimated: $\Delta p/p \ll 1$ (allows considering a given input energy/momentum)
- **target**: (fixed target $\cong$ macroscopic sample)
  - consists often of a large number of particles B (e.g., H-gas in a container, stack of lead plates, etc.)

- or an impurity potential in a solid (dislocations, vacancies, and other irregularities of the ion lattice)

- **Elastic scattering**:

$$A + B \to A + B$$

Same particles in the initial and final states, i.e., total kinetic energy is conserved

- **Inelastic scattering**: final state particles $\neq$ initial state particles, or the structure of A,B can change.

- For example:

$$\underset{\text{positron}}{e^+} + \underset{\text{hydrogen in its ground state}}{H} \to \underset{\text{final state}}{X}$$

X could be for example

(i) $e^+ + H$: elastic scattering

(ii) $e^+ + H^*$: excitation of H

(iii) $e^+ + p + e^-$: ionization of H

(iv) $p + 2\gamma$: annihilation

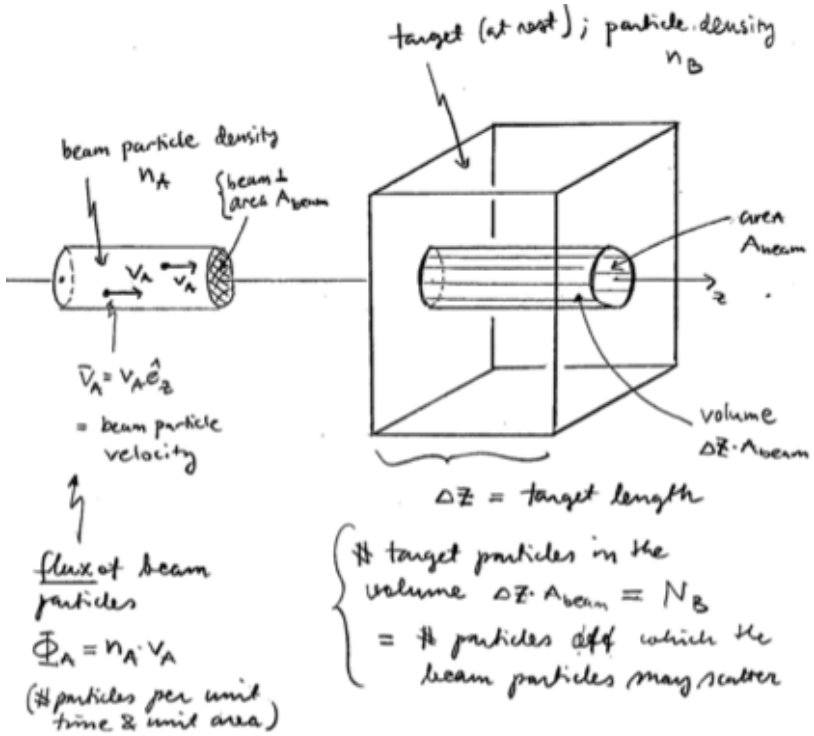
(v) $p + (e^+e^-)$: positronium formation

(ii)-(v) are inelastic

- What is measured in the final state: $p = |\mathbf{p}|$, θ, φ (possibly polarization, spin, etc.)

- Key quantity: **Cross section** for a scattering $A+B \to C+D+\cdots$ = number of these scattering events per unit time, per one target particle B, divided by the flux of incoming beam particles A

- Illustrate:



- Observed: n_S = number of scattering events in a unit time
- obviously, the more flux Φ_A and the larger N_B, the larger must n_S be:

$$\boxed{n_S = \sigma \Phi_A N_B} \tag{1}$$

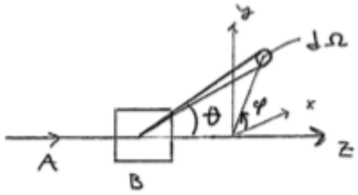
  where σ is an effective "cross section" which the beam particles see. It is also related to the probability for the scattering to happen. These have the physical units:

$$\begin{aligned} [n_S] &= 1/\text{time} \\ [\Phi_A] &= 1/(\text{time} \cdot \text{length}^2) \\ [N_B] &= 1 \\ [\sigma] &= \text{length}^2. \end{aligned}$$

- We can therefore define the **scattering cross section** as

$$\boxed{\sigma = \frac{n_S}{\Phi_A N_B} = \frac{n_S}{n_A v_A n_B \Delta z A}} \tag{2}$$

- Units used in nuclear and particle physics: $[\sigma] = 1$ b $= 1$ barn $= 10^{-28}$ m^2 $= 100$ fm^2
- n_S depends on the scattering process considered, i.e., on the probability of scattering, i.e., on the strength and range of the interaction and the beam energy

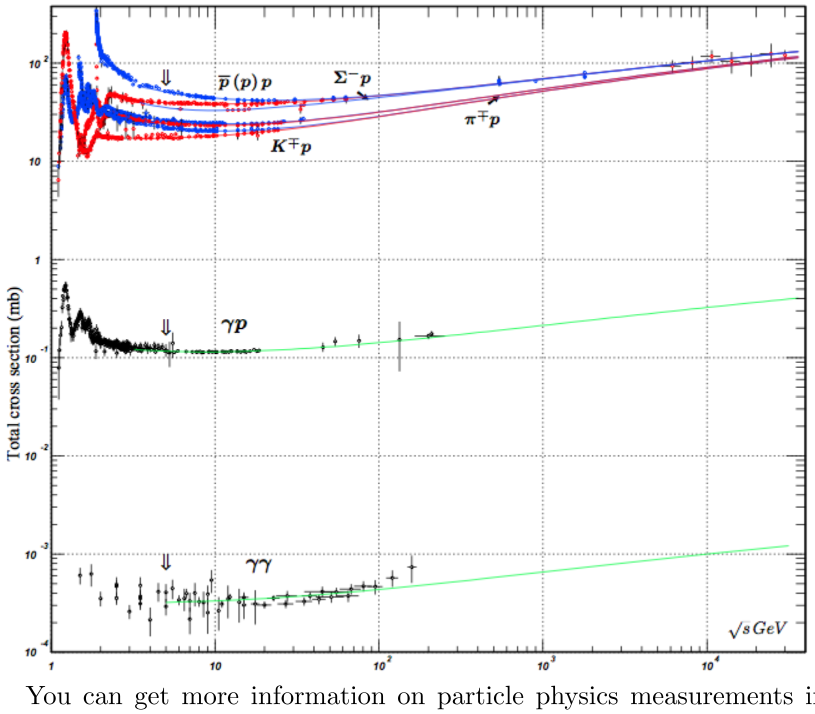


- **Total cross section** of an A+B scattering = $\sigma_{\rm tot}(AB \to X) = \sigma_{\rm el} + \sigma_{\rm in}$, where X is any final state
- **Elastic cross section** of an A+B scattering = $\sigma_{\rm el}(AB \to AB)$
- **Inelastic cross section** of an A+B scattering = $\sigma_{\rm in}(AB \to X \neq AB)$
- **Differential cross section**

$$\frac{d\sigma}{d\Omega} = \frac{n_S(\theta,\varphi)}{\Phi_A N_B},$$

where $dn_S = n_S(\theta,\varphi)d\Omega$ is the number of particles per unit time, scattered into the infinitesimal solid angle $d\Omega$.

Total cross section example from particle physics (source: K. Nakamura, et al., Review of Particle Physics, J. Phys. G: Nucl. Part. Phys. **37**, 075021 (2010).)



You can get more information on particle physics measurements in the course FYSH300 Particle Physics.

In this chapter, we aim to

(i) Formulate the **general 3d scattering problem**, where the wave function far away from the scattering region satisfies

$$\psi(\mathbf{r}) = \underbrace{Ae^{ikz}}_{\text{incoming}} + \underbrace{f(\theta,\varphi)\frac{e^{ikr}}{r}}_{\text{outgoing}}.$$

The rest of the chapter deals with methods aiming to solve $f(\theta, \varphi)$.

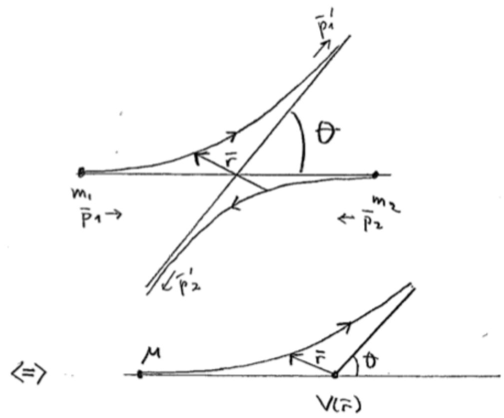
(ii) We use the Green's function technique to transform the Schrödinger equation to an **integral equation**. This is then solved with the **Born approximation**. It is especially useful for weak potentials, where the deviation of the particle's initial trajectory is small.

(iii) The hand-written notes also contain a description of the **partial wave analysis**, where the θ dependence is expanded in terms of the spherical harmonics. This method is useful especially for low-energy particles (compared to the potential strength), since for that case $f(\theta)$ is a weak function of θ. However, in this year's course that part is not included, but in case you are interested, you may browse through the corresponding notes.

Alternatively to the lecture notes, you may also follow Ch. 11 in Griffiths' book.

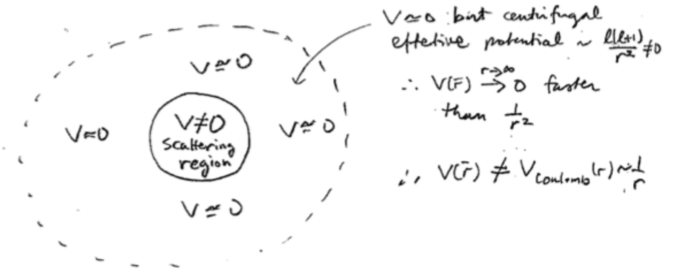
II.2 Formulation of the 3d scattering problem: boundary conditions of the wave function, cross section, optical theorem

We consider here the elastic scattering of two spinless, nonrelativistic particles. In laboratory frame both of them may have a finite momentum, whereas in the center-of-momentum (CMS) frame one of them (the "target") can be fixed:

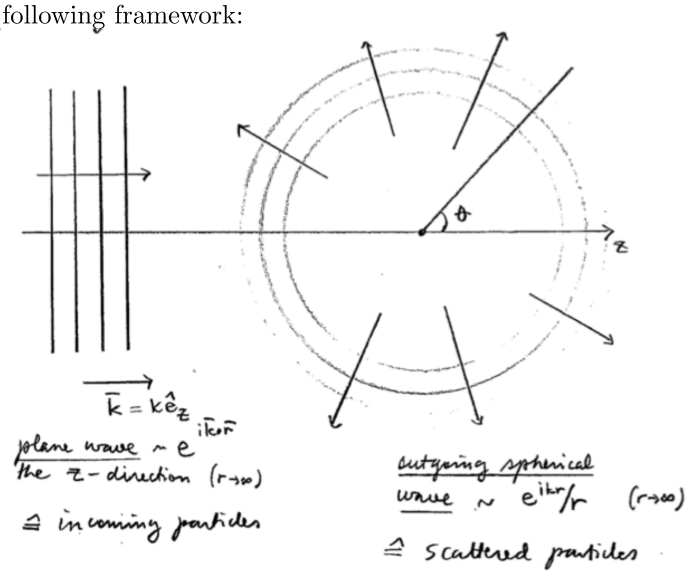


In the CMS frame the total momentum of the system vanishes, and hence $\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_1' + \mathbf{p}_2' = 0$, the relevant energy is the relative kinetic energy between the particles, and the relevant position is the relative position, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. This is equivalent to a scattering of a particle of a reduced mass $\mu = m_1 m_2/(m_1 + m_2)$ of a potential $V(\mathbf{r})$.

In order to be able to calculate the cross section, we must assume a **finite-range**, localized (and often spherically symmetric) potential $V = V(\mathbf{r})$; $r^3 V(\mathbf{r}) \xrightarrow{r\to\infty} 0$:



We proceed analogously to what was done in QM I in the case of a 1D problem (Griffiths, Ch. II). Instead of using calculationally much more difficult wave packets and their time evolution to describe particles and their motion, we assume a **stationary** situation, i.e., that the beam has been "turned on" already for a while and that we thus have a steady flux of incoming and scattered particles. This "turning on" is described in more detail in Ch. III. We thus consider the scattering problem within the following framework:



That is, at $r \to \infty$, the particles behave as free, $V(r \to \infty) \to 0$.

Let us first specify the **incoming plane wave** in the 3d case, far away from the scattering center $\mathbf{r} = 0$. The stationary Schrödinger equation reads in the position representation

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

This is solved with the plane wave solution (prefactor comes from the properties of Fourier transformation)

$$\boxed{\Psi(\mathbf{r}) = \frac{1}{(2\hbar)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad k^2 = \frac{2\mu E}{\hbar^2}}$$

This is hence the form of the wave function for the beam of particles far away from the scattering center.

For a radially symmetric potential, we can make the separating Ansatz $\psi(\mathbf{r}) = R(r)Y_{lm}(\Omega)$ (see Griffiths, Ch. IV). There, $R(r)$ satisfies the radial Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\partial_r(r^2\partial_r) + \underbrace{\frac{\hbar^2 l(l+1)}{2\mu r^2}}_{\text{This one remains}} + \underbrace{V(r)}_{\to 0 \text{ as } r\to 0} \right] R(r) = ER(r),$$

i.e., we assume $V(r)$ to decay faster than the centrifugal term $l(l+1)/r^2$ at large r. In other words,

$$\boxed{r^2R''(r) + 2rR'(r) + [(kr)^2 - l(l+1)]R(r) = 0}$$

The general solution to this can be specified in terms of spherical Bessel ($j_l(x)$) and Neumann ($n_l(x)$) functions:

$$R(r) = Aj_l(kr) + Bn_l(kr)$$

For large arguments, they have the asymptotic behavior

$$\begin{aligned} j_l(x) &\xrightarrow{x\gg l(l+1)/2} \frac{1}{x}\sin(x - l\pi/2) = \frac{1}{x}\frac{1}{2i}\left(e^{i(x-l\pi/2)} - e^{-i(x-l\pi/2)}\right) \\ n_l(x) &\xrightarrow{x\gg l(l+1)/2} -\frac{1}{x}\cos(x - l\pi/2) = -\frac{1}{x}\frac{1}{2}\left(e^{i(x-l\pi/2)} + e^{-i(x-l\pi/2)}\right) \end{aligned}$$

For a large r, the solution to the radial equation can hence be written in terms of plane waves:

$$\boxed{R(r) \xrightarrow{kr\to\infty} \frac{1}{2kr}\left[\left(\frac{A}{i} - B\right)e^{-il\pi/2}\underbrace{e^{ikr}}_{\substack{\text{outgoing}\\ \text{wave?}}} + \left(-\frac{A}{i} - B\right)e^{il\pi/2}\underbrace{e^{-ikr}}_{\substack{\text{incoming}\\ \text{wave?}}}\right]}. \tag{3}$$

Identification in terms of incoming and outgoing waves can be done by considering the probability flux, or **probability current density**

$$\boxed{\mathbf{j} = -\frac{i\hbar}{2\mu}\left[\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - (\nabla\Psi^*(\mathbf{r}))\Psi(\mathbf{r})\right] = \frac{\hbar}{\mu}\mathrm{Im}[\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r})]}.$$

This can be derived from the general continuity equation defining a relation between the probability density and probability current density.[1]

[1] See a separate video describing this.

Continuity equation and quantum current density
Generally in physics current densities can be defined in terms of the **continuity equation** relating the current density j and the corresponding density ρ (say, charge density, particle density, probability density,...)

$$\boxed{\frac{d\rho}{dt} + \nabla \cdot \mathbf{j} = 0} \tag{4}$$

The continuity equation basically states that spatial variations in the current are accompanied by changes (in time) of the density, or in other words, time-dependent changes in density result into spatial dependence of the current.

Now consider the probability density in quantum mechanics, i.e.,

$$\rho(\mathbf{r}) = |\Psi(\mathbf{r})|^2,$$

Its time derivative satisfies

$$\begin{aligned}\frac{d}{dt}|\Psi|^2 &= (\psi \partial_t \Psi^* + \Psi^* \partial_t \Psi) \\ &= \frac{i}{\hbar}(\Psi H^* \Psi^* - \Psi^* H \Psi)\end{aligned}$$

Now use the position representation of the Hamiltonian, $H = -\hbar^2\nabla^2/(2m) + V(\mathbf{r})$. The potential commutes with $\rho(\mathbf{r})$ and hence can be dropped. Moreover, we can use

$$\Psi \nabla^2 \Psi^* - \Psi^* \nabla^2 \Psi = \nabla \cdot (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi).$$

As a result, we get

$$\frac{d}{dt}|\Psi|^2 = -\frac{i\hbar}{2m}\nabla \cdot (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi) \equiv -\nabla \cdot \mathbf{j}.$$

We hence found an expression for the current density in terms of the wave function

$$\boxed{\mathbf{j} = \frac{i\hbar}{2m}(\Psi \nabla \Psi^* - \Psi^* \nabla \Psi) = \frac{\hbar}{m}\mathrm{Im}(\Psi^* \nabla \Psi).} \tag{5}$$

For the plane wave solution describing the incoming wave, $\psi_{\text{in}} = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}$, we get

$$\boxed{\mathbf{j}_{\text{in}} = +\frac{1}{(2\pi)^3}\frac{\hbar \mathbf{k}}{\mu}}$$

In defining the cross section, we need the amount (per unit time) of scattered particles moving through a sphere surface at $r \to \infty$:

$$n = \int \underbrace{\mathbf{d}S}_{r^2 d\Omega \hat{e}_r} = r^2 \int d\Omega \underbrace{j_r}_{\text{radial component of flux}} .$$

Recall the spherical harmonics representation of gradient: $\nabla = \hat{e}_r\partial_r + \hat{e}_\theta\partial_\theta/r + \hat{e}_\varphi\partial_\varphi$ so that

$$j_r = \frac{\hbar}{\mu}\text{Im}[\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r})]_r = \frac{\hbar}{\mu}\text{Im}[R^*(r)R'(r)Y^*_{lm}(\Omega)Y_{lm}(\Omega)].$$

From Eq. (3), we hence want to see what happens with $R(r) = Ce^{\pm ikr}/r$. Direct calculation:

$$n = r^2\frac{\hbar}{\mu}|C|^2\text{Im}\left[\frac{e^{\mp ikr}}{r}\cdot\frac{e^{\pm ikr}}{r}(\pm ik - \frac{1}{r})\underbrace{\int d\Omega Y^*_{\text{lm}}(\Omega)Y_{\text{lm}}(\Omega)}_{=1}\right] = \pm|C|^2\frac{\hbar k}{\mu}.$$

The total particle flux is thus independent of the radial coordinate r, which is desired because there are no sources of sinks of particles. Now we can identify what the signs mean:
"+" $\cong$ outgoing spherical wave
"-" $\cong$ incoming spherical wave
Moreover, we find that the proper asymptotic behavior of an outgoing spherical wave is e^{ikr}/r.

Now we are in position of defining the quantum scattering problem:

Quantum scattering problem
With a potential $V = V(\mathbf{r})$ decaying faster than $1/r^2$, find the solutions of the spherical Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

or

$$\boxed{(\nabla^2 + k^2)\Psi(\mathbf{r}) = U(\mathbf{r})\Psi(\mathbf{r}), \quad \text{where } U(\mathbf{r}) \equiv \frac{2\mu}{\hbar}V(\mathbf{r})}$$

fulfilling the boundary condition

$$\boxed{\Psi(\mathbf{r}) \xrightarrow{r\to\infty} \frac{1}{(2\pi)^{3/2}}\left[\underbrace{e^{i\mathbf{k}\cdot\mathbf{r}}}_{\substack{\text{incoming}\\ \text{particles}}} + \underbrace{\frac{e^{ikr}}{r}f_k(\theta,\varphi)}_{\substack{\text{spherical outgoing wave}\\ \cong\text{ scattered particles}}}\right]} \tag{6}$$

Here

$$\boxed{f_k(\theta,\varphi) = \text{ scattering amplitude}}$$

We have two remaining problems: what is $f_k(\theta,\varphi)$ if $V(\mathbf{r})$ is known? What is the relation between $f_k(\theta,\varphi)$ and the scattering cross section σ?

Note that $f_k(\theta, \varphi)$ is a generalization of the transmission and reflection probability amplitudes from the one-dimensional scattering problem.

To answer the question posed above, let us check the particle fluxes for our Ansatz asymptotic wave function, Eq. (6). The total flux is

$$\begin{aligned}
\mathbf{j} =& \frac{\hbar}{\mu}\mathrm{Im}[\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r})] = \mathbf{j}_{\mathrm{in}} + \mathbf{j}_{\mathrm{scatt}} + \mathbf{j}_{\mathrm{int}} \\
\overset{r\to\infty}{=}& \frac{\hbar}{\mu}\mathrm{Im}[\underbrace{\Psi^*_{\mathrm{in}}(\mathbf{r})\nabla\Psi_{\mathrm{in}}(\mathbf{r})}_{\propto\mathbf{j}_{\mathrm{in}}} + \underbrace{\Psi^*_{\mathrm{scatt}}(\mathbf{r})\nabla\Psi_{\mathrm{scatt}}(\mathbf{r})}_{\propto\mathbf{j}_{\mathrm{scatt}}} \\
&+ \underbrace{\Psi^*_{\mathrm{in}}(\mathbf{r})\nabla\Psi_{\mathrm{scatt}}(\mathbf{r}) + \Psi^*_{\mathrm{scatt}}(\mathbf{r})\nabla\Psi_{\mathrm{in}}(\mathbf{r})}_{\propto\mathbf{j}_{\mathrm{int}}}].
\end{aligned}$$

Therefore, we find that the total current consists of three parts. The first of these is nothing but the flux of incoming particles, denoted Φ_A in Eq. (1). To understand the second, let us consider the number of particles scattered into a solid angle $d\Omega$ in a unit time per target particle

$$\frac{dn_S}{N_B} = \frac{1}{N_B}n_S(\theta,\varphi)d\Omega \overset{r\to\infty}{=} \mathbf{d}S\cdot\mathbf{j}_{\mathrm{scatt}} = r^2 d\Omega (j_{\mathrm{scatt}})_r.$$

Here

$$\mathbf{j}_{\mathrm{scatt}} = \frac{\hbar}{\mu}\mathrm{Im}[\Psi^*_{\mathrm{scatt}}(\mathbf{r})\nabla\Psi_{\mathrm{scatt}}(\mathbf{r})] = \frac{1}{(2\pi)^3}\frac{\hbar}{\mu}\mathrm{Im}\left[\frac{e^{-ikr}}{r}f_k^*(\Omega)\nabla\left(\frac{e^{ikr}r}{f_k(\Omega)}\right)\right].$$

In other words,

$$(\mathbf{j}_{\mathrm{scatt}})_r = \frac{1}{(2\pi)^3}|f_k(\Omega)|^2\frac{\hbar k}{\mu}\frac{1}{r^2}.$$

and therefore

$$\frac{n_S}{N_B} = r^2 d\Omega(\mathbf{j}_{\mathrm{scatt}})_r = \frac{1}{(2\pi)^3}|f_k(\theta,\varphi)|^2\frac{\hbar k}{\mu}d\Omega.$$

We can hence define the cross section as in Eq. (2),

$$\sigma = \frac{n_S}{\Phi_A N_B} = \frac{1}{\Phi_A}\frac{\int n_S(\theta,\varphi)d\Omega}{N_B}$$

yielding

$$\boxed{\sigma = \int d\Omega |f_k(\theta,\varphi)|^2} \quad \text{elastic cross section} \tag{7}$$

and

$$\boxed{\frac{d\sigma}{d\Omega} = |f_k(\theta,\varphi)|^2} \quad \text{differential cross section} \tag{8}$$

We have thus answered the second question above: finding the (absolute value of the) scattering amplitude $f_k(\theta, \varphi)$ amounts to calculating the differential cross section. In retrospect it is quite clear that the two quantities must contain the same information, because they are the only ingredients left open after specifying the scattering setup!

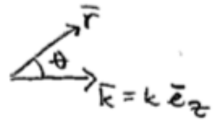
Before proceeding to the methods to calculate $f_k(\theta,\varphi)$, let us fix one loose end: what happens to the interference current term $\mathbf{j}_{\text{in}}$? It is given by[2]

[2] There is also a video derivation on this.

$$\mathbf{j}_{\text{int}} \overset{r\to\infty}{=} \frac{\hbar}{\mu}\text{Im}[\Psi_{\text{in}}^*\nabla\Psi_{\text{scatt}} + \Psi_{\text{scatt}}^*\nabla\Psi_{\text{in}}]$$
$$= \frac{\hbar}{\mu}\frac{1}{(2\pi)^3}\text{Im}[e^{-i\mathbf{k}\cdot\mathbf{r}}\nabla(\frac{e^{ikr}}{r}f_k(\Omega)) + \frac{e^{-ikr}}{r}f_k^*(\Omega)\nabla e^{i\mathbf{k}\cdot\mathbf{r}}].$$

Its radial component becomes

$$(\mathbf{j}_{\text{int}})_r = \frac{\hbar}{\mu}\frac{1}{(2\pi)^3}\text{Im}\left[e^{-ikr\cos(\theta)}f_k(\Omega)\underbrace{\partial_r\frac{e^{ikr}}{r}}_{\frac{e^{ikr}}{r}(ik-1/r)} + \frac{e^{-ikr}}{r}f_k^*(\Omega)\underbrace{\partial_r e^{ikr\cos(\theta)}}_{ik\cos(\theta)e^{ikr\cos(\theta)}}\right],$$



where we *defined* the spherical angle θ by the relation $\mathbf{k}\cdot\mathbf{r} = kr\cos(\theta)$.

Proceeding, we get

$$(\mathbf{j}_{\text{int}})_r \overset{r\to\infty}{=} \frac{\hbar}{\mu}\frac{1}{(2\pi)^3}\text{Im}\left[\frac{ik}{r}(f_k(\theta,\varphi)e^{ikr(1-\cos(\theta))} + \text{complex conjugate}) + o\left(\frac{1}{r^2}\right)\right].$$

Now, when $\theta \neq 0 \to 1-\cos(\theta) \neq 0$, $e^{ikr(1-\cos\theta)}$ oscillates very rapidly when $r\to\infty$.

So far we have assumed that the incoming beam is entirely monoenergetic, i.e., contains only a single wave vector. This certainty of momentum would correspond to a wave packet with an infinite spread in space. In reality, the beam is never monoenergetic, but contains some spread $\Delta k \ll k$ in the wave number. This spread is not very relevant for the incoming and outgoing currents, but it matters in the case of the very rapidly oscillating interference current. Therefore, let us average over this spread with some weight function $g(k)$. That means that when we compute the flux across a spherical surface at $r\to\infty$, we should replace

$$\int \mathbf{d}S\cdot\mathbf{j} = r^2\int d\Omega j_r(r,\theta,\varphi;k) \mapsto r^2\int d\Omega\int dk g(k) j_r(r,\theta,\varphi;k),$$

where $g(k)$ is a smooth function of k, with a spread Δk around some maximal value of k. Generally $g(k)$ is set by the experiment in question.

This means that now we have integrals of the type[3]

[3] For example, a Gaussian weight function $g(k)f_k = C\exp[-((k-k_0)/\Delta k)^2]$ gives an integral $\propto$ $r\exp\{-[(1-\cos\theta)(\Delta k)r]^2/4\}$, which vanishes when $r\to\infty$.

$$\lim_{r\to\infty}\int dk \underbrace{g(k)kf_k}_{\text{smooth in k}}\exp(ikr\underbrace{(1-\cos\theta)}_{\neq 0}) = 0$$

Therefore, the oscillating terms appearing at $\theta \neq 0$ vanish. Therefore, let us include only the integration near $\theta \sim 0$:

$$\begin{aligned}
\int \mathbf{d}S \cdot \mathbf{j} &\simeq \frac{\hbar}{\mu} \frac{1}{(2\pi)^3} r^2 \int_0^{2\pi} d\varphi \int_{1-\cos\theta}^{1} d(\cos\theta) \mathrm{Im}[\frac{ik}{r}(f_k(0) e^{ikr(1-\cos(\theta))} + \text{complex conj.})\\
&= \frac{\hbar}{\mu} \frac{1}{(2\pi)^3} 2\pi r^2 \mathrm{Im}[\frac{e^{ikr}}{-ikr}|_{1-\cos\theta}^{1} d(\cos\theta) e^{-ikr\cos(\theta)} + c.c. + o(1/r^2)]\\
&= \frac{\hbar}{\mu} \frac{1}{(2\pi)^3} 2\pi r^2 \mathrm{Im}[\frac{i}{r^2}(i f_k(0)\{1 - e^{ikr\cos(\delta\theta)}\} + c.c.) + o(1/r^2)]\\
&= -\frac{\hbar}{\mu} \frac{1}{(2\pi)^3} 2\pi \mathrm{Im}[f_k(0) - f_k^*(0) + o(1/r^2)]\\
&= -\frac{\hbar}{\mu} \frac{1}{(2\pi)^3} 4\pi \mathrm{Im}[f_k(0)] + o(1/r^2).
\end{aligned}$$

So what is the consequence of this lengthy calculation? Recall the continuity equation

$$\partial_t \rho(t, \mathbf{r}) + \nabla \cdot \mathbf{j} = 0,$$

where ρ is the (probability or particle) density. In the stationary case the first term vanishes, and the continuity equation is a statement of probability flux conservation. In other words,

$$\begin{aligned}
0 &= \int_{\substack{\text{sphere of}\\ \text{radius } R}} d^3\mathbf{r} \nabla \cdot \mathbf{j} \overset{\text{Gauss}}{=} \int_{\substack{\text{surface of}\\ R\text{-sphere}}} \mathbf{d}S \cdot \mathbf{j} = R^2 \int d\Omega \hat{j}_r\\
&= R^2 \int d\Omega [(j_{\text{in}})_r + (j_{\text{scatt}})_r + (j_{\text{int}})_r].
\end{aligned}$$

The incoming current satisfies $(j_{\text{in}})_r = (2\pi)^{-3}\hbar k/\mu(\hat{e}_z)_r = (2\pi)^{-3}\hbar k/\mu \cos(\theta)$ and therefore

$$\int d\Omega (j_{\text{in}})_r \propto \int_{-1}^{1} d(\cos(\theta)) \cos(\theta) = 0.$$

In other words, the incoming current brings in (say, from the left) equally much current as they take out (say, to the right). On the other hand, the scattered total current is

$$R^2 \int d\Omega (j_{\text{scatt}})_r = \frac{1}{(2\pi)^3} \frac{\hbar k}{\mu} \underbrace{\int d\Omega |f_k(\Omega)|^2}_{\sigma_{\text{tot}}}.$$

Combining the continuity equation and our result for the interference current, we get the **optical theorem**

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k} \mathrm{Im}[f_k(\theta = 0)]} \tag{9}$$

According to the optical theorem, which we have now derived, the total cross section is related to the imaginary part of the forward scattering amplitude. Physically, this means that behind the target, at $\theta \to 0$, the incoming wave and the scattered wave interfere destructively, so that the intensity of the beam which has passed the target decreases by an amount which is proportional to the total cross section.

II. 3. Integral equation for (potential) scattering

After having specified the scattering problem (see page 23), we should try to solve it at least in some particular cases. In other words, we wish to solve the 3d differential equation

$$(\nabla^2 + k^2)\Psi(\mathbf{r}) = U(\mathbf{r})\Psi(\mathbf{r}) \tag{10}$$

with the asymptotic boundary condition

$$\Psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow{r\to\infty} \frac{1}{(2\pi)^{3/2}}\left(e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f_k(\theta,\varphi)\right).$$

Note that here the vector $\mathbf{k}$, $k \equiv |\mathbf{k}|$ is some quantity specified for the problem. In particular, the direction of the vector $\mathbf{k}$ specifies a reference direction.

To solve the problem, let us first define

(i) The solution $\phi_{\mathbf{k}}(\mathbf{r})$ of the homogeneous ($U = 0$) equation:

$$(\nabla^2 + k^2)\phi_{\mathbf{k}}(\mathbf{r}) = 0; \quad \phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

(ii) **Green's function** $G_{\mathbf{k}}(\mathbf{r},\mathbf{r}')$ satisfying

$$(\nabla^2 + k^2)G_{\mathbf{k}}(\mathbf{r},\mathbf{r}') = \delta^{(3)}(\mathbf{r}-\mathbf{r}').$$

Equation (10) can now be cast in the form of an **integral equation**:[4]

$$\boxed{\Psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^3\mathbf{r}' G_{\mathbf{k}}(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')} \tag{11}$$

[4]Check this: $(\nabla^2 + k^2)\Psi_{\mathbf{k}} = (\nabla^2 + k^2)\phi_{\mathbf{k}} + \int d^3\mathbf{r}(\nabla^2 + k^2)G_{\mathbf{k}}(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}') = U(\mathbf{r})\Psi_{\mathbf{k}}(\mathbf{r})$.

We wish to use this integral equation to help find a general scheme for solving the scattering problem. This is done below, but before we manage to do so, we need to discuss the Green's function in more detail.

Green's functions do not only depend on the differential equation, but also on the boundary conditions. Now, in order to fulfill the boundary conditions of the scattering problem, $\phi_{\mathbf{k}}(\mathbf{r})$ has to be taken to be the incoming plane wave, and we have to **define** the Green's function suitably, so that

$$\int d^3\mathbf{r}' G_{\mathbf{k}}(\mathbf{r},\mathbf{r}')U(\mathbf{r})\Psi_{\mathbf{k}}(\mathbf{r}') \xrightarrow{r\to\infty} \frac{e^{ikr}}{r} f_k(\theta,\phi),$$

i.e., it should correspond to the outgoing spherical wave.

Let us make a Fourier expansion of $G_{\mathbf{k}}$, by assuming that it only depends on the difference of its arguments:

$$G_{\mathbf{k}}(\mathbf{r},\mathbf{r}') = G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}') = \int \frac{d^3\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} g_{\mathbf{k}}(\mathbf{q}).$$

It satisfies

$$(\nabla^2+k^2)G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}') = \int \frac{d^3\mathbf{q}}{(2\pi)^3}(k^2-q^2)e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}g_{\mathbf{k}}(\mathbf{q}) = \delta^{(3)}(\mathbf{r}-\mathbf{r}') = \int \frac{d^3\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}$$

or

$$(k^2-q^2)g_{\mathbf{k}}(\mathbf{q}) = 1.$$

In order to compute $G_{\mathbf{k}}$, we need to consider k in the complex plane,[5] $k \mapsto k + i\epsilon$, and set $\epsilon \to 0$ at the end of the calculation. But how should it tend to 0, from positive or negative values? As a matter of fact, the choice of the sign of ϵ determines different Green's functions.

[5] Why? Patience: the motivation comes below.

We hence have $g_{\mathbf{k}}(\mathbf{q}) = ((k+i\epsilon)^2 - q^2)^{-1}$, and

$$\begin{aligned}
G_{\mathbf{k}}(\mathbf{r}) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{(k+i\epsilon)^2-q^2} \\
&= \frac{1}{(2\pi)^3}\int_0^\infty \frac{dqq^2}{(k+i\epsilon)^2-q^2}\int_0^{2\pi} d\varphi \underbrace{\int_{-1}^{1} d\cos\theta e^{iqr\cos\theta}}_{(e^{iqr}-e^{-iqr})/(iqr)} \\
&= \frac{2\pi}{(2\pi)^3}\frac{1}{ir}\int_0^\infty \frac{dqq}{(k+i\epsilon)^2-q^2}(e^{iqr}-e^{-iqr}) \\
&= \frac{2\pi}{(2\pi)^3}\frac{1}{ir}\int_{-\infty}^\infty \frac{dqqe^{iqr}}{(k+i\epsilon)^2-q^2}.
\end{aligned}$$

We get $G_{\mathbf{k}}(\mathbf{r}) = I_k(r)/(4\pi^2 ri)$, where

$$I_k(r) = \int_{-\infty}^{\infty} dq \frac{qe^{iqr}}{(k+i\epsilon)^2-q^2}. \tag{12}$$

This integral can be computed as an integral in the complex q-plane, using the **residue theorem**. This means that we need to introduce some mathematical machinery that comes handy in various physics problems, but especially those dealing with Green's functions.

II.3.1 Functions of complex variable and their integration

Let us start by the definition of a complex derivative[6]

[6] The whole section is explained also in a series of videos in Koppa.

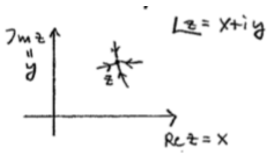


Fig. 3 $f'(z)$ should be independent of the direction of h.

$$\boxed{f'(z) \equiv \lim_{h\to 0}\frac{f(z+h)-f(z)}{h}; f, z, h \in \mathbb{C}}$$

This should be "isotropic", i.e., independent of the direction of h as in Fig. 3. In other words,

$$\begin{aligned}
f'(z) &= \lim_{\Delta x\to 0}\frac{f(z+\Delta x)-f(z)}{\Delta x} = \frac{\partial f}{\partial x} \\
&= \lim_{i\Delta y\to 0}\frac{f(z+i\Delta y)-f(z)}{i\Delta y} = -i\frac{\partial f}{\partial y}.
\end{aligned}$$

Let us separate the real and imaginary parts of $f(z) = u(z) + iv(z)$, where $u, v \in \mathbb{R}$, $z = x + iy$. Then

$$f'(z) = \frac{\partial f}{\partial x} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}$$

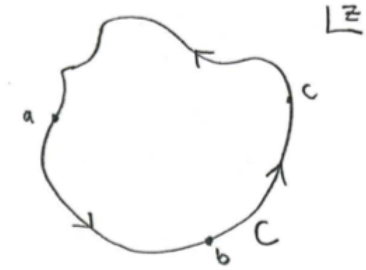
and

$$f'(z) = -i\frac{\partial f}{\partial y} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}.$$

Equating the real and imaginary parts separately yields

$$\boxed{\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} = 0 \text{ and } \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0} \tag{13}$$

These are known as the **Cauchy-Riemann equations**.



Contour integrals (viivaintegraalit)

Consider a closed path C in the complex plane. Let us moreover define the *winding direction* to be counterclockwise (arrows in the figure). The contour integral along C can be defined in parts,

$$\oint_C dz f(z) = \int_{C(a\to b)} f(z) + \int_{C(b\to c)} f(z) + \int_{C(c\to a)} f(z) = -\oint_C dz f(z).$$

Let $f(z)$ to be **analytic** on and within C above.[7] Consider the contour integral along C:[8]

$$\begin{aligned}\oint_C dz f(z) &= \oint_C (dx + idy)(u + iv) = \oint_C (udx - vdy) + i\oint_C (vdx + udy) \\ &= \oint \underbrace{(u\hat{e}_x - v\hat{e}_y)}_{\mathbf{A}} \cdot \mathbf{d}x + i\oint_C \underbrace{(v\hat{e}_x + u\hat{e}_y)}_{\mathbf{B}} \cdot \mathbf{d}x \\ &\overset{\text{Stokes theorem}}{=} \int_{S_c} da\, \underbrace{\hat{e}_3 \cdot (\nabla \times \mathbf{A})}_{(\nabla\times\mathbf{A})_3} + i\int_{S_c} da\, \underbrace{\hat{e}_3 \cdot (\nabla \times \mathbf{B})}_{(\nabla\times\mathbf{B})_3} \\ &= \int_{S_c} da(-\partial_x v - \partial_y u) + i\int_{S_c} da(\partial_x u - \partial_y v) = 0.\end{aligned}$$

The last result was obtained by using the Cauchy-Riemann equations (13): both integrands vanish. In other words,

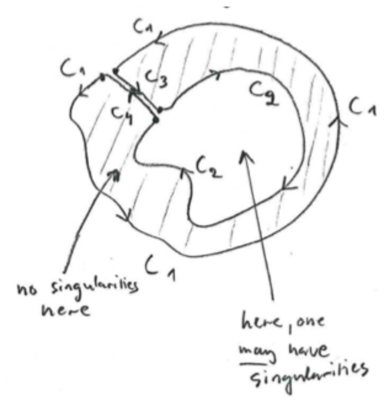
$$\boxed{\oint dz f(z) = 0}$$

This results allows us to state the

Cauchy's integral theorem
A contour integral of a complex function $f(z)$ over a closed and simply connected (no holes) region C vanishes if $f(z)$ is analytic on C and

[7] This means that Taylor series $\sum_{n=0}^{N} \frac{f^{(n)}(a)}{n!}(z - a)^n$ tends to $f(z)$ as $N \to \infty$ for each z inside the area spanned by C.

[8] On the second line, consider $\mathbf{d}x$ as a three-vector: $\mathbf{d}x = (dx, dy, dx_3)$ with some extra coordinate dx_3.



within its interior. In other words, $f(z)$ has no singularities inside or on C.

Now let us start *transforming the contour*. For example, take $C = C_1 + C_3 + C_2 + C_4$ as in the figure. Assume that there are no holes or singularities within C, i.e., the shaded region in the figure. Then, Cauchy's integral theorem states that

$$0 = \oint_C dz f(z) = \Bigg(\oint_{C_1} + \oint_{C_2} + \underbrace{\int_{C_3} + \int_{C_4}}_{\substack{\text{cancel, opposite} \\ \text{directions}}} \Bigg) dz f(z) = \oint_{C_1} dz f(z) + \oint_{C_2} dz f(z).$$

Changing the direction in C_2 this then yields

$$\oint_{C_1} dz f(z) = \oint_{C_2} dz f(z).$$

In this way, we can "shrink" the contours.[9]

[9] The area spanned by C_2 is smaller than that of C_1, but the value of the integral is the same - and not necessarily zero!

We can generalize this result to many loops, which may contain singularities at $z_1, z_2, \dots, z_n$:

$$\boxed{\oint_C dz f(z) = \sum_{n=1}^{\infty} \oint_{C_n} dz f(z)}$$

Note that all contours run in the counterclockwise direction.

Suppose now that $f(z)$ has an **isolated singularity** at $z = z_0$. This means that $f(z)$ is analytic in the area surrounding z_0 but not exactly at $z = z_0$. By the definition of analyticity, $f(z)$ **cannot** be written in terms of its Taylor series. Rather, we have to use the **Laurent series** of $f(z)$

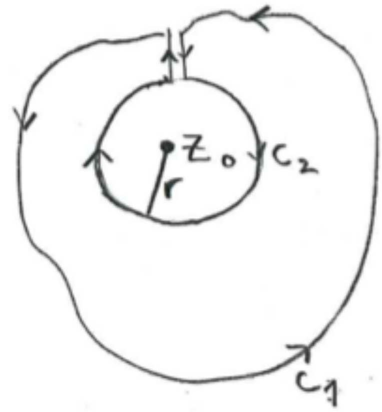
$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n. \tag{14}$$

Let us assume there is an $m \in \mathbb{Z}$, $m > 0$ so that $a_{n<-m} = 0$. Then

$$f(z) = \underbrace{\frac{a_{-m}}{(z-z_0)^m} + \frac{a_{-m+1}}{(z-z_0)^{m+1}} + \cdots + \frac{a_{-1}}{z-z_0}}_{\text{singular terms}}$$
$$+ \underbrace{a_0 + a_1(z-z_0) + a_2(z-z_0)^2 + \cdots}_{\text{analytic}}.$$

Above, we call
z_0 a **pole of order** m
a_{-1} the **residue** of $f(z)$ at $z = z_0$

$$\boxed{a_{-1} = \operatorname*{Res}_{z=z_0} f(z)}$$



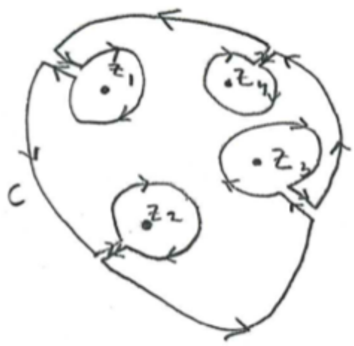
Let $f(z)$ now have a pole of order m at $z = z_0$,

$$f(z) = \sum_{n=-m}^{\infty} a_n (z - z_0)^n.$$

Take C_2 as a circle around z_0

$$\boxed{z - z_0 = re^{i\varphi}}$$

i.e., $dz = ire^{i\varphi} d\varphi$, $\varphi \in [0, 2\pi]$. The contour integral becomes



$$\begin{aligned}\oint_{C_1} dz f(z) = \oint_{C_2} dz f(z) &= \sum_{n=-m}^{\infty} a_n \oint_{C_2} dz \underbrace{(z - z_0)^n}_{r^n e^{in\phi}} \\ &= i \sum_{n=-m}^{\infty} a_n r^{n+1} \qquad \underbrace{\int_0^{2\pi} d\varphi e^{i(n+1)\varphi}}_{2\pi\delta_{n,-1}:\text{only } n=-1 \text{ survives!}} \\ &= 2\pi i a_{-1} = 2\pi i \operatorname*{Res}_{z=z_0} f(z).\end{aligned}$$

This result can be generalized to the case of many singularities at $z_1, z_2, \ldots$

$$\boxed{\oint_{C_1} dz f(z) = 2\pi i \sum_{j=1}^{n} \operatorname*{Res}_{z=z_j} f(z)} \tag{15}$$

We have derived the **Residue theorem**, a very important result.
The residues can be obtained from

(i) Expanding $f(z)$ as a Laurent series and taking the coefficient a_{-1} or, more easily,

(ii) using a pocket formula for a pole of order n (can be verified trivially)

$$\boxed{\operatorname*{Res}_{z=z_0} f(z) = \lim_{z \to z_0} \frac{1}{(n-1)!} \left(\frac{d}{dz}\right)^{n-1} [(z - z_0)^n f(z)]}$$

In the quite often encountered special case of a simple pole $m = 1$ at $z = z_0$ we have

$$f(z) = \frac{a_{-1}}{(z - z_0)} + a_0 + \cdots$$

and

$$\operatorname*{Res}_{z=z_0} f(z) = \lim_{z \to z_0} (z - z_0) f(z).$$

Let us now use these results for the evaluation of the Green's function.

II.3.2 Evaluation of the Green's function

We can finally come back to our initial problem that we reached on page 28. We would like to calculate

$$I_k(r) = \int_{-\infty}^{\infty} dq \underbrace{\frac{qe^{iqr}}{(k+i\epsilon)^2 - q^2}}_{f(q)} .$$

Since $(k+i\epsilon)^2 - q^2 = (k+i\epsilon-q)(k+i\epsilon+q)$, the **poles** of $f(q)$ are at $k+i\epsilon-q=0$ and $k+i\epsilon+q=0$, or

$$\boxed{q = k+i\epsilon \equiv q_+} \text{ and } \boxed{q = -k-i\epsilon \equiv q_- = -q_+}$$

and since

$$f(q) = \frac{-qe^{iqr}}{(q-q_+)(q-q_-)} = -\frac{qe^{iqr}}{q_+ - q_-}\left(\frac{1}{q-q_+} - \frac{1}{q-q_-}\right),$$

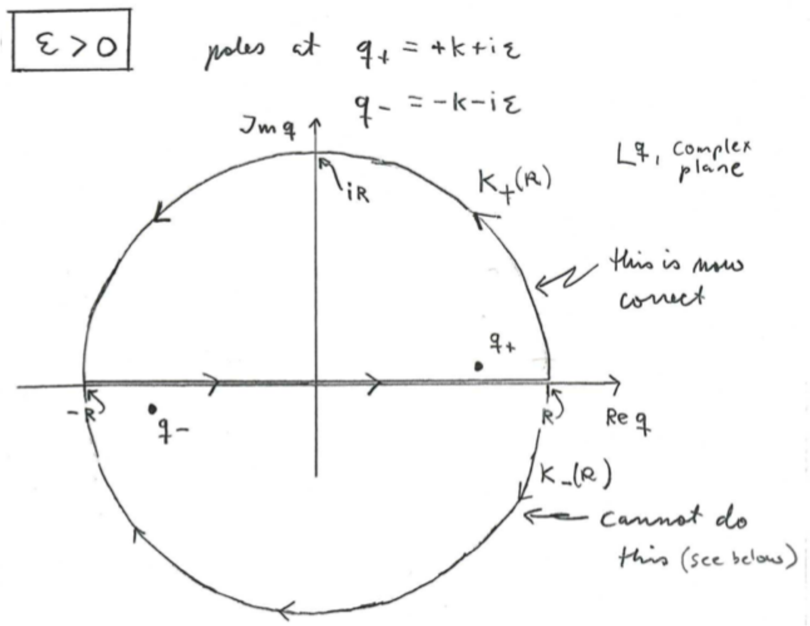
the poles at $q = q_\pm$ are **simple poles** of order 1. Let us calculate the residues:

$$\operatorname*{Res}_{q=q_\pm} f(q) = \lim_{q\to q_\pm} \frac{(-q)e^{iqr}}{(q-q_+)(q-q_-)} = \frac{-q_\pm e^{iq_\pm r}}{\underbrace{q_\pm - q_\mp}_{=2q_\pm}}$$

$$= -\frac{1}{2}e^{iq_\pm r}.$$

These are the **residues** of $f(q)$ at $q = q_\pm$.

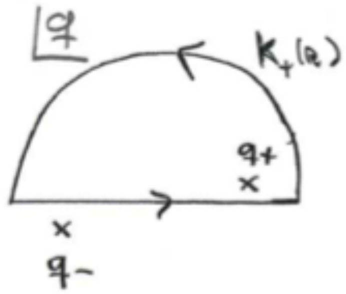
Wait! We have a simple integral over real values of q. Where is the contour? The trick is to *consider* the integral over the real axis as part of a closed contour that closes along the complex plane as shown in the following picture (where we have chosen $\epsilon > 0$):



We should hence "close" the contour along the upper or lower complex half-plane. But which one should we use? This we see below. Either way, we can see that one of the poles is inside the contour C, and the other one is outside. Anyway, the idea is the following: the residue theorem says

$$2\pi i \underbrace{\operatorname*{Res}_{q=q_k}}_{\text{poles inside } C} f(q) = \oint_C dq f(q)$$

$$= \lim_{R\to\infty}\left[\int_{-R}^{R} dq f(q) + \underbrace{\int}_{\substack{K_+(R) \text{ or } K_-(R)\\ \text{semicircle at } |q|=R}} dq f(q)\right].$$



The first term inside the square brackets is the one we wish to compute. Now our aim is to **choose** the contour $K_+(R)$ or $K_-(R)$ so that the second integral vanishes. Let us choose first $K_+(R)$, i.e., close the contour in the upper half-plane. In this case, the pole q_+ is inside C, and q_- is outside it. In other words,

$$\int_{-\infty}^{\infty} dq f(q) = 2\pi i \operatorname*{Res}_{q=q_+} f(q) - \lim_{R\to\infty}\int_{K_+(R)} dq f(q).$$

For $q \in K_+(R)$, we can set $q = Re^{i\varphi}$, $\varphi \in [0,\pi]$. Let us show that the contour integral along $K_+(R)$ vanishes as $R \to \infty$. We have[10]

$$f(q \in K_+(R)) = \frac{-Re^{i\varphi}e^{iRr\cos(\varphi)}e^{-Rr\sin(\varphi)}}{R^2e^{i2\varphi} - (k+i\epsilon)^2}$$

$$= \frac{-e^{i(-\varphi+Rr\cos\varphi)}}{R(1-(q_+/R)^2e^{-i2\varphi})}e^{-Rr\sin(\varphi)}.$$

Now take the limit $R \to \infty$. The absolute value of $f(q = Re^{i\varphi})$ tends to

$$|f(q = Re^{i\varphi})| \xrightarrow{R\to\infty} \frac{1}{R}\exp[-\underbrace{Rr\sin\varphi}_{\substack{\geq\ 0 \text{ since}\\ \varphi\in[0,\pi]}}] \to 0.$$

The integral along contour $K_+(q)$ running along the upper half-plane therefore vanishes.[11] We can see why we have to close the contour C through the upper half plane, as for $K_-(R)$ we would have $q = Re^{-i\varphi}$ (again $\varphi \in [0,\pi]$) and

$$e^{iqr} \overset{q=Re^{-i\varphi}}{=} e^{iRr\cos\varphi}\exp[+\underbrace{Rr\sin\varphi}_{\substack{\geq\ 0 \text{ since}\\ \varphi\in[0,\pi]}}] \xrightarrow{R\to\infty} \infty!$$

The integral along the lower half-plane would hence **not** vanish for $R \to \infty$.

In general which half-plane to close the contour depends on the case. For exponential functions with poles in the upper half-plane, we can

[10] $e^{iqr} = e^{iRre^{i\varphi}} = e^{iRr(\cos\varphi + i\sin\varphi)} = e^{iRr\cos\varphi}e^{-Rr\sin\varphi}$

[11] Note that the length of the contour is πR, and thus increases linearly with an increasing R. However, the integrand vanishes exponentially with increasing R. Exponential function wins a linear function, and thus the result vanishes.

prove the **Jordan's lemma**:

If $|g(z)| \leq M(R)$, when $|z| = R$, Im $z > 0$ (upper half-plane), and $M(R) \xrightarrow{R\to\infty} 0$, then

$$\lim_{R\to\infty} \int_{K_+(R)} g(z)e^{ikz} = 0$$

Proof:[12]

[12] Use here $z = Rei\varphi$ and thus $dz = iRe^{i\varphi}d\varphi$.

$$\int_{K_+(R)} g(z)e^{ikz} = \int_0^{\varphi} d\varphi iRe^{i\varphi} g(Re^{i\varphi})e^{+ikR\cos\varphi}e^{-kR\sin\varphi}$$

$$\Rightarrow |\int_{K_+(R)} g(z)e^{ikz}| \leq \int_0^{\pi} d\varphi |iRe^{i\varphi}g(Re^{i\varphi})\underbrace{e^{-ikR\cos\varphi}}_{\text{phase, } |.|=1} e^{-kR\sin(\varphi)}|$$

$$= R\int_0^{\varphi} |g(Re^{i\varphi})|e^{-kR\sin(\varphi)}$$

$$\overset{|g(z)|\leq M(R)}{\leq} RM(R)\int_0^{\varphi} d\varphi e^{-kR\sin\varphi} = 2RM(R)\int_0^{\pi/2} d\varphi e^{-kR\sin\varphi}$$

$$\overset{\sin\varphi\geq 2\varphi/\pi}{\leq} 2RM(R)\int_0^{\pi/2} d\varphi e^{-kR2\varphi/\pi}$$

$$= 2RM(R)\frac{\pi}{2kR}(1-e^{-kR}) = \frac{\pi M(R)}{k}(1-e^{-kR}) \xrightarrow[M(R)\to 0]{R\to\infty} 0.\square$$

Now let us apply Jordan's lemma to our problem:

$$f(q) = \underbrace{\frac{-q}{q^2-(k+i\epsilon)^2}}_{g(q)} e^{iqr},$$

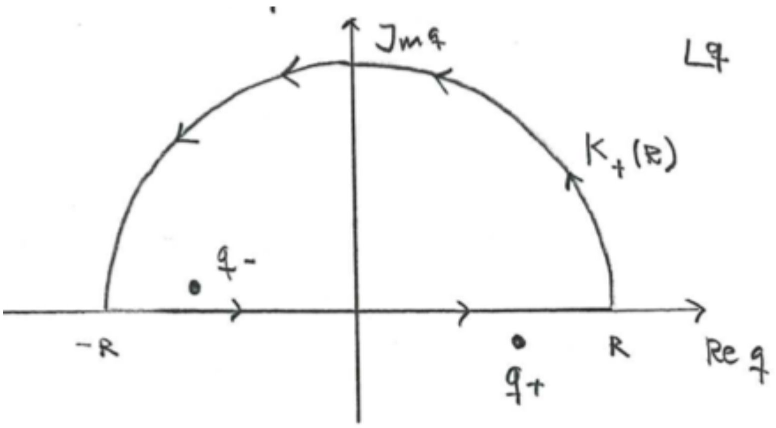
and we have that $|g(Re^{i\varphi})| = R^{-1}|1-(q/R)^2e^{-i2\varphi}|^{-1} \leq 1/R = M(R) \to 0$, so it fulfills the assumptions. This means that as $R \to \infty$, the integral of $f(q)$ of the contour $K_+(R)$ over the upper half-plane vanishes. Moreover, from Eq. (12) we have for $\epsilon > 0$

$$I_k^{\epsilon>0}(r) = \int_{-\infty}^{\infty} dq f(q) = 2\pi i \operatorname*{Res}_{q=q_+} f(q) = 2\pi i(-\frac{1}{2}e^{iq_+r}) = -\pi i e^{i(k+i\epsilon)r}.$$

In other words, the Green's function is

$$\boxed{G_{\mathbf{k}}^{\epsilon>0}(\mathbf{r}) = \frac{I_k^{\epsilon>0}}{4\pi^2 ri} = -\frac{1}{4\pi}\frac{e^{i(k+i\epsilon)r}}{r} \xrightarrow{\epsilon\to 0^+} -\frac{1}{4\pi}\frac{e^{ikr}}{r}} \qquad (16)$$

Let us quickly check what would happen with the choise $\epsilon < 0$. In this case the pole at $q_+ = k + i\epsilon = k - i|\epsilon|$ would be outside C and the pole q_- inside it:



Now you should show that we get

$$I_{\mathbf{k}}^{\epsilon<0} = 2\pi i(-\frac{1}{2}e^{iq_- r}) = -\pi i e^{-i(k+i\epsilon)r}$$

and the corresponding Green's function would be

$$G_{\mathbf{k}}^{\epsilon<0}(\mathbf{r}) = -\frac{1}{4\pi}\frac{e^{-ikr}}{r}$$

In other words,

$$G_{\mathbf{k}}^{\epsilon\to 0\pm}(\mathbf{r}) = -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}.$$

Next, we show that it is $+\epsilon$ that we want for the scattering problem, to describe an outgoing spherical wave.

II.3.3 Integral equation for potential scattering (IEPS)

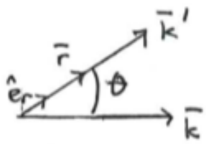
Now, finally, substitute the above Green's function back to the integral equation (11), still allowing for either sign of ϵ. We get

$$\boxed{\Psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) - \frac{1}{4\pi}\int d^{(3)}\mathbf{r}'\frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')} \qquad (17)$$

Here $U(\mathbf{r}') \neq 0$ in some vicinity of $\mathbf{r}' \approx 0$. We should check the boundary condition at $r \to \infty$ (not $r' \to \infty$) and choose the Green's function (+ or

-) accordingly. Therefore, we should assume $r' \ll r \to \infty$, and expand:

$$\begin{aligned} k|\mathbf{r}-\mathbf{r}'| &= k\sqrt{(\mathbf{r}-\mathbf{r}')^2} = kr\sqrt{1-\frac{2\mathbf{r}\cdot\mathbf{r}'}{r^2}+\underbrace{\left(\frac{r'}{r}\right)^2}_{\to 0}} \\ &\approx kr\left(1-\frac{1}{2}2\underbrace{\frac{\mathbf{r}}{r}}_{\hat{e}_r}\cdot\frac{\mathbf{r}'}{r}+o\left(\left(\frac{r'}{r}\right)^2\right)\right) \\ &= kr-\underbrace{k\hat{e}_r}_{\equiv\mathbf{k}'}\cdot\mathbf{r}'. \end{aligned}$$



Note that we identified (defined) here the wave vector of the scattered particle, $\mathbf{k}' \equiv k\hat{e}_r$. As we are describing elastic scattering (energy of the incoming particle equals that of the outgoing particle), it has the same magnitude as the incoming particle, but a different direction.

Inserting this expansion into Eq. (17) yields in the lowest order

$$\Psi_{\mathbf{k}}(\mathbf{r}) \overset{r\to\infty}{=} \phi_{\mathbf{k}}(\mathbf{r}) - \frac{e^{\pm ikr}}{r}\frac{1}{4\pi}\int d^3\mathbf{r}' e^{\mp i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}').$$

Comparing this to the desired form, Eq. (6), we find that in order to get the proper behavior, we have to *choose* in the Green's function $\epsilon \to 0^+$.

Now recall that

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}}.$$

Moreover, comparing to the boundary condition (6), we can find an expression for the scattering amplitude

$$f_k(\theta,\varphi) = -\frac{(2\pi)^{3/2}}{4\pi}\int d^{(3)}\mathbf{r}' \underbrace{e^{-i\mathbf{k}'\cdot\mathbf{r}'}}_{(2\pi)^{3/2}\phi^*_{\mathbf{k}'}(\mathbf{r}')} U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')$$

or

$$\boxed{f_k(\theta,\varphi) = -2\pi^2\int d^{(3)}\mathbf{r}'\phi^*_{\mathbf{k}'}(\mathbf{r}')U(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')} \tag{18}$$

This we need for the calculation of the differential scattering cross section.

II.4. Solving the IEPS: Born approximation

Let us then solve the IEPS via **an iteration method**, using the fact that Eq. (17) contains $\Psi_{\mathbf{k}}(\mathbf{r})$ on both sides of the equation. Let us hence substitute the left hand side to the right hand side. We get

$$\begin{aligned} \Psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) &+ \int d^{(3)}\mathbf{r}' G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}')U(\mathbf{r}')\phi(\mathbf{k}') \\ &+ \int d^{(3)}\mathbf{r}' d^{(3)}\mathbf{r}'' G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}')U(\mathbf{r}')G_{\mathbf{k}}(\mathbf{r}'-\mathbf{r}'')U(\mathbf{r}'')\Psi_{\mathbf{k}}(\mathbf{r}''). \end{aligned}$$

Substituting $\Psi_{\mathbf{k}}(\mathbf{r})$ repeatedly to this equation hence generates the **Born series** of $\Psi_{\mathbf{k}}(\mathbf{r})$

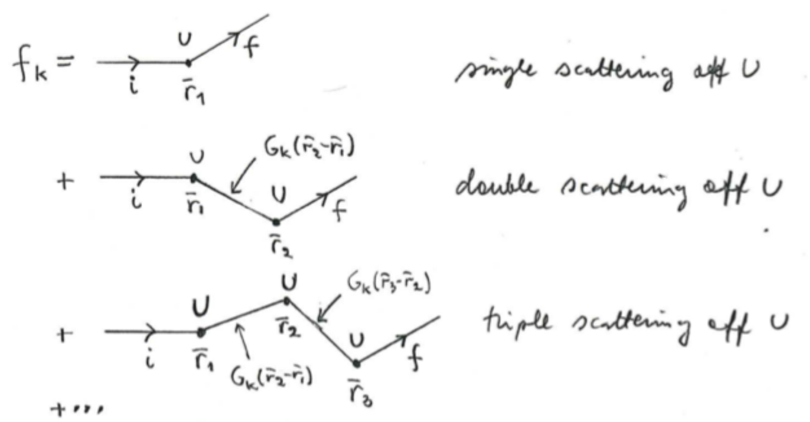
$$\Psi_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^{(3)}\mathbf{r}' G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}')U(\mathbf{r}')\phi(\mathbf{k}') + \int d^{(3)}\mathbf{r}' d^{(3)}\mathbf{r}'' G_{\mathbf{k}}(\mathbf{r}-\mathbf{r}')U(\mathbf{r}')G_{\mathbf{k}}(\mathbf{r}'-\mathbf{r}'')U(\mathbf{r}'')\phi_{\mathbf{k}}(\mathbf{r}'') + \ldots .$$

Note that each new term contains a higher-order power of $U = 2\mu V/(\hbar^2)$. It is hence an *expansion* in U.

Let us write the scattering amplitude in a similar series. For illustration, let us define the wave vector of the incoming particle or "initial state wave vector" by $\mathbf{k}_i \equiv \mathbf{k} = k\hat{e}_z$ and that of the outgoing particle or "final state wave vector" by $\mathbf{k}_f \equiv \mathbf{k}' = k\hat{e}_r$. The Born series of the scattering amplitude is

$$\begin{aligned} f_k(\theta,\varphi) =& -2\pi^2 \int d^{(3)}\mathbf{r}_1 \phi^*_{\mathbf{k}_f}(\mathbf{r}_1)U(\mathbf{r}_1)\Psi_{\mathbf{k}_i}(\mathbf{r}_1) \\ =& -2\pi^2 \int d^{(3)}\mathbf{r}_1 \phi^*_{\mathbf{k}_f}(\mathbf{r}_1)U(\mathbf{r}_1)\phi_{\mathbf{k}_i}(\mathbf{r}_1) \\ & -2\pi^2 \int d^{(3)}\mathbf{r}_1 d^{(3)}\mathbf{r}_2 \phi^*_{\mathbf{k}_f}(\mathbf{r}_2)U(\mathbf{r}_2)G_{\mathbf{k}}(\mathbf{r}_2-\mathbf{r}_1)U(\mathbf{r}_1)\phi_{\mathbf{k}_i}(\mathbf{r}_1) \\ & -2\pi^2 \int d^{(3)}\mathbf{r}_1 d^{(3)}\mathbf{r}_2 d^{(3)}\mathbf{r}_3 \phi^*_{\mathbf{k}_f}(\mathbf{r}_3)U(\mathbf{r}_3)G_{\mathbf{k}}(\mathbf{r}_3-\mathbf{r}_2)U(\mathbf{r}_2)G_{\mathbf{k}}(\mathbf{r}_2-\mathbf{r}_1)U(\mathbf{r}_1)\phi_{\mathbf{k}_i}(\mathbf{r}_1) + o(U^4). \end{aligned}$$

We can interpret this graphically and physically as follows:



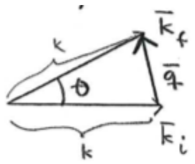
The Green's function $G_{\mathbf{k}}(\mathbf{r}_i - \mathbf{r}_j)$ is also called the **propagator**, which describes the propagation of a free particle from $\mathbf{r}_j$ to $\mathbf{r}_i$. The interpretation of the Born series is thus that f_k consists of a series of processes containing $n = 1, 2, 3, \ldots$ scattering events, where the incoming particle scatters off U at $\mathbf{r}_1$, after which it moves as a free particle to the point $\mathbf{r}_2$, where it scatters off U again, and so on. Obviously, if U is very weak relative to the incident energy $E = \hbar^2 k^2/(2\mu)$ of the scattering particle(s), the contribution from multiple scatterings to the total scattering amplitude is small. In this case only the first term in the Born series is of relevance.

It can be shown[13] that the Born series converges for all k, if $U(\mathbf{r})$ does not have bound states, i.e., $U(\mathbf{r})$ is weak enough, and for (sufficiently) large k, if $U(r) \xrightarrow{r\to\infty} 1/r^p$, where $p > 3$ and $U(r) \xrightarrow{r\to 0} 1/r^s$, where $s < 2$. We can then define the

[13] Klein and Lee, Nuovo Cimento **10**, 1078 (1958). The exact assumptions are here for your interest, you don't need to remember them.

Born approximation = the first term in the Born series for $f_k(\Omega)$

$$f_B(\theta,\varphi) = -2\pi^2 \int d^{(3)}\mathbf{r}\phi^*_{\mathbf{k}_f}(\mathbf{r})U(\mathbf{r})\phi_{\mathbf{k}_i}(\mathbf{r}) = -\frac{1}{4\pi}\int d^{(3)}\mathbf{r}e^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{r}}U(\mathbf{r}). \quad (19)$$



Let us examine this further by defining the **momentum exchange vector**

$$\hbar\mathbf{q} = \hbar(\mathbf{k}_f - \mathbf{k}_i)$$

By straightforward trigonometry (see the picture) one can show that

$$\frac{q}{2} = k\sin\frac{\theta}{2}$$

Note that the momentum exchange vector depends on the angle θ. Using q we can hence write the Born approximated form of the scattering amplitude in terms of the Fourier transform of the potential

$$\tilde{U}(\mathbf{q}) \equiv \mathcal{F}[U(\mathbf{r})] = \frac{1}{(2\pi)^{3/2}}\int e^{-i\mathbf{q}\cdot\mathbf{r}}U(\mathbf{r})$$

and hence

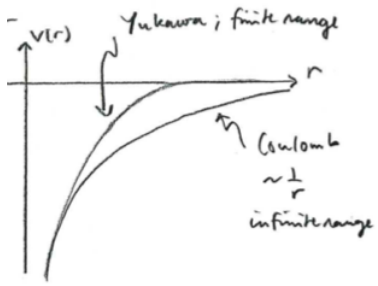
$$f_B(\theta,\varphi) = -\frac{1}{4\pi}\int d^{(3)}\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}U(\mathbf{r}) = -\frac{(2\pi)^{3/2}}{4\pi}\tilde{U}(\mathbf{q})$$

For a **spherically symmetric** potential, $V(\mathbf{r}) = V(r)$ we have[14]

[14] We made a similar type of an integral on page 28.

$$f_B(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int \underbrace{d^{(3)}\mathbf{r}_1}_{d\cos\theta_1 d\varphi_1 r_1^2 dr_1} \exp(-i \underbrace{\mathbf{q}\cdot\mathbf{r}_1}_{qr_1\cos(\theta_1)})$$

$$= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}4\pi\int_0^\infty dr_1 r_1^2 V(r_1)\frac{1}{qr_1}\sin(qr_1).$$



So, for a spherically symmetric potential we have

$$f_B(\theta,\varphi) \overset{V(\mathbf{r})=V(r)}{=} f_B(\theta) = -\frac{2\mu}{\hbar^2}\int_0^\infty dr rV(r)\frac{\sin(qr)}{q}$$

Remember that the θ-dependence is in $q = 2k\sin\frac{\theta}{2}$.

Example 0.1 Yukawa potential

$$V(r) = v_0\frac{e^{-\kappa r}}{r}$$

The potential thus has a range $1/\kappa$. It described a **screened** Coulomb potential, massive photons, or for example serves as a crude model for the nuclear binding force in an atomic nucleus. The benefit of it is that it leads to easy integrals using elementary functions. In the exercises you will show that for the Yukawa potential

$$f_B(\theta,\varphi) = -\frac{2\mu v_0}{\hbar^2}\frac{1}{q^2+\kappa^2} = -\frac{2\mu v_0}{\hbar^2}\frac{1}{4k^2\sin^2\frac{\theta}{2}+\kappa^2}.$$

The differential cross section for elastic scattering off a Yukawa potential becomes in the Born approximation

$$\frac{d\sigma}{d\Omega} = |f_B(\theta,\varphi)|^2 = \frac{4\mu^2 v_0^2}{\hbar^4}\frac{1}{(4k^2\sin^2\frac{\theta}{2}+\kappa^2)^2}.$$

For curiosity, let us take the limit $\kappa \to 0$, and set $v_0 = q_1 q_2/(4\pi\epsilon_0)$ as in the Coulomb potential, recalling that $k^2 = 2\mu E/\hbar^2$. We thus get[15]

$$\frac{d\sigma}{d\Omega}|_{\kappa\to 0} = \left[\frac{q_1 q_2}{16\pi\epsilon_0 E\sin^2\frac{\theta}{2}}\right]^2 = \frac{d\sigma}{d\Omega}|_{\text{Rutherford}}$$

[15] The same result is obtained both classically and quantum mechanically, see Griffiths' book, page 415 for more discussion.

Notice, however, that if we take the limit $\kappa \to 0$, we are stepping outside the validity region of the above approach, since the range of V_{Coulomb} is infinite. In particular, integrating the above differential cross section over the angles yields $\sigma_{\text{Coulomb}} = \infty$. However, the above result for the differential cross section is nevertheless correct.

Phew! There are a lot of technical details in the above sections. What should you take along? Well, at least

- Definition of the scattering problem, total and differential cross section
- Quantum scattering problem and the scattering amplitude
- Green's function and integral equation
- Solving the scattering Green's function: small imaginary term into wave number; residue theorem (complex integration)
- Using residue theorem to evaluate certain types of integrals
- Once we have the Green's function, for "weak enough" potentials we can solve the scattering problem via Born series
- Note how the Born approximated version couples to the scattering amplitude.