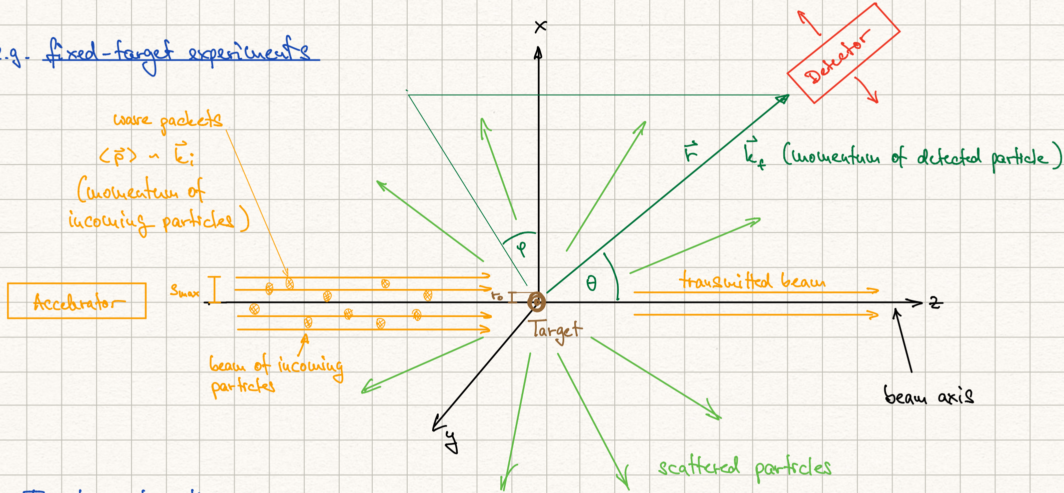
Chapter 2: Scattering Theory

2.1. Basics

→ Scattering experiments: One of the most important type of experiment to learn about the inner structure of matter and materials

↳ e.g. crystal lattice, atomic structure, nucleon structure modern high-energy particle physics } ↳ structures too small to study otherwise

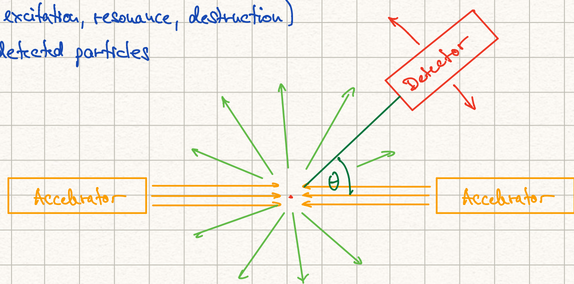
e.g. fixed-target experiments



↳ Two types of scattering processes:

(a) Elastic scattering: particles in the incoming beam = detected particles
$|\vec{k}_i| = |\vec{k}_f|$, $E_i = E_f$

(b) Inelastic scattering: target get changed (excitation, resonance, destruction)
incoming particles ≠ detected particles
$|\vec{k}_i| \neq |\vec{k}_f|$



Big high energy collider experiments:

Large Hadron Collider (CERN, 2008 - 2035)
proton-proton (pp)

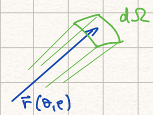
International Linear Collider (?) (Japan, ~ 2030 - ?): electron-positron ($e^- e^+$)

Large Electron-Positron Collider (LEP, CERN 1989-2000): $e^+ e^-$

Tevatron (Fermilab, Chicago, 1983-2011): proton-antiproton ($p\bar{p}$)

Principles:

- momentum of incoming particles very well known : $\vec{k}_i$
- intensity of incident beam very well known
- measurement of scattered particles at distance $|\vec{r}|$ from target at solid angle element $d\Omega(\theta,\varphi)$ with respect to beam axis : $\vec{k}_f$, particle kind, intensity



$e^{ipx} = 2\pi$
$x = \frac{2\pi}{p}$

→ Aim: Draw conclusions on :
- interactions, forces between particles
- inner structure of particles (resolution $\sim \lambda_{\vec{k}_i} = \frac{2\pi}{|\vec{k}_i|}$)

Scale hierarchies : → Basic properties of all scattering experiments

$|\vec{r}|$: (makroscopic) distance between target and detector ($\sim 1\,cm - 10\,m$)
S_{max} : width of the beam, "beam size" ($\sim 10\,nm = 10^{-8}\,m$ for modern colliders)
r_0 : size of target $\simeq$ range of interaction
($\sim 10^{-10}\,m$ — $10^{-15}\,m$ — $10^{-17}\,m$ → ...)
(atomic radius) (nucleon radius) (weak interaction range)
$\sim (1\,keV)^{-1}$ $\sim (1\,GeV)^{-1}$ $\sim (100\,GeV)$

} → implies: potential $V(r)$ falls faster than $\frac{1}{r}$ for $r \gg r_0$

$$\boxed{\text{strong scale hierarchy : } |\vec{r}| \gg S_{max} \gg r_0}$$
→ approximations that are essential for the concept of scattering

$1\,keV = 10^3\,eV$
$1\,MeV = 10^6\,eV$
$1\,GeV = 10^9\,eV$
$1\,TeV = 10^{12}\,eV$

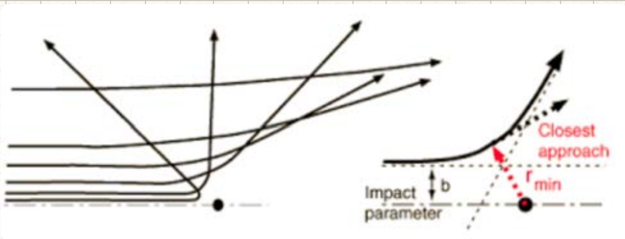
→ Rule of thumb : ($\hbar = c = 1$) $2 \cdot 10^{-16}\,m = (1\,GeV)^{-1}$

typical energies : mass of the electron : $m_e = 0.5\,MeV$
$m_{proton} \simeq m_{neutron} \simeq 1\,GeV$
$M_{goldatom} \simeq M_{topquark} \simeq 175\,GeV$
Center of mass energy @ LHC : $13\,TeV = 13000\,GeV$
Planck Scale : $10^{19}\,GeV$
↖ energy where space-time becomes discontinuous
scale of quantum gravity

For most scattering experiments an actual scattering ($\theta > 0$) is quite rare. Most of the time nothing happens and the incoming particle emerges in the transmitted beam.

→ We consider this case usually.

2.2. Classic Potential Scattering



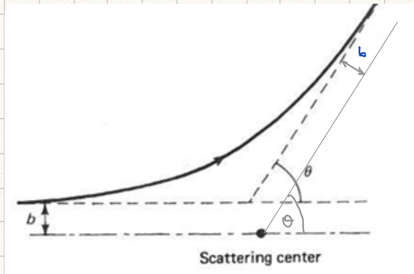


Fig. 6.1 Scattering from a fixed potential: θ is the scattering angle and b is the impact parameter.

Assumption: Potential is only r-dependent : $V = V(r)$ $\Rightarrow$ φ-independence (azimuth)

b : impact parameter
θ : scattering angle
} unique relation between θ and b that depends on the form of $V(r)$ $\Rightarrow$ $\theta = \theta(b)$

Example: Scattering off a hard sphere

$\rightarrow$ $V(r) = \begin{cases} 0, & r > R \\ \infty, & r < R \end{cases}$ $\qquad 0 \leq \theta \leq \pi$

We have: $b = R \sin\alpha$, $2\alpha + \theta = \pi$

$\Rightarrow \sin\alpha = \sin\left(\frac{\pi - \theta}{2}\right) = \cos\left(\frac{\theta}{2}\right)$, $b = R\cos\left(\frac{\theta}{2}\right)$

$$\Rightarrow \theta(b) = \begin{cases} 2\arccos\left(\frac{b}{R}\right), & b \leq R \\ 0, & b > R \end{cases}$$

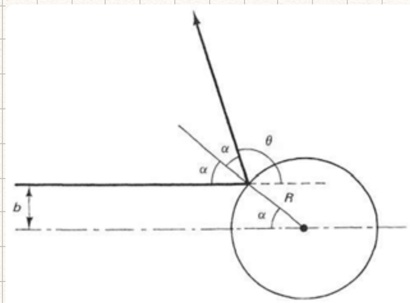


Fig. 6.2 Hard-sphere scattering.

$\rightarrow$ Differential Cross Section: $\frac{d\sigma}{d\Omega}$

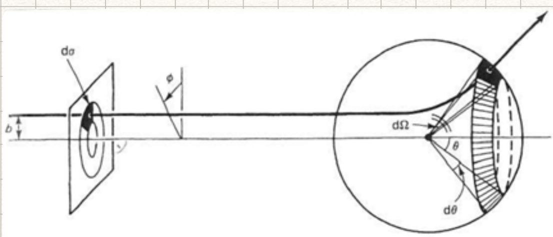


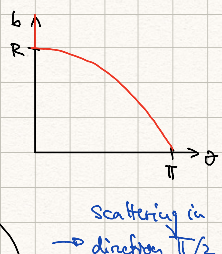
Fig. 6.3 Particle incident in area dσ scatters into solid angle dΩ.

$\rightarrow$ All particles that enter through area segment $d\sigma(\theta, \phi)$ are scattered into the solid angle segment $d\Omega(\theta, \phi)$. $\qquad \varphi = \phi$

$\rightarrow$ We have: $d\sigma = b \, db \, d\phi$

$d\Omega = \sin\theta \, d\theta \, d\phi$

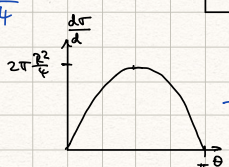
$$\Rightarrow \frac{d\sigma}{d\Omega}(\theta, \phi) = \left| \frac{b \, db \, d\phi}{\sin\theta \, d\theta \, d\phi} \right| = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$



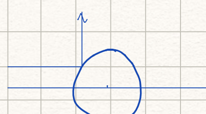
For hard sphere: $\frac{db}{d\theta} = -\frac{R}{2}\sin\left(\frac{\theta}{2}\right)$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{R^2}{2} \frac{\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)}{\sin(\theta)} = \frac{R^2}{4}$$

$\rightarrow$ $\frac{d\sigma}{d\theta} = \frac{R^2}{4} 2\pi \sin\theta$



$\rightarrow$ scattering in direction $\pi/2$ most frequent



↳ **Total Cross Section : σ**

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega \qquad \int d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, \sin\theta = \int_0^{2\pi} d\phi \int_{-1}^{+1} d\cos\theta$$

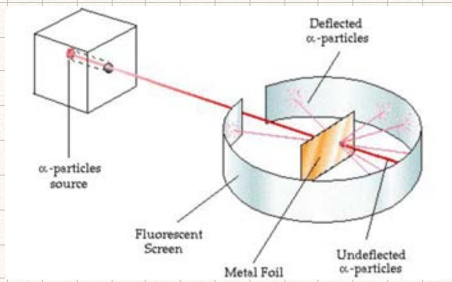
By definition: Particles that are not scattered (i.e. scattering angle $\theta = 0$) do not contribute to the total cross section.

→ effective area that leads to scattering

For hard sphere: $\sigma = \int d\Omega \frac{R^2}{4} = \frac{R^2}{4} 4\pi = R^2 \pi$

↖ as expected

Example : Rutherford Scattering



→ Scattering of a particle with electr. charge q_1 off a Coulomb potential of a stationary particle with el. charge q_2: $V(r) = \frac{1}{4\pi} \frac{q_1 q_2}{r}$

→ Rutherford : Fixed-target experiment
beam of α particles shot on nuclei of gold atoms

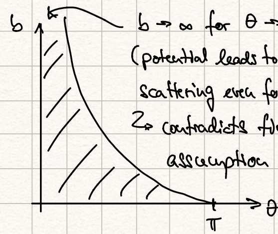
↳ classical mechanics : $b = \frac{q_1 q_2}{8\pi E} \cot\left(\frac{\theta}{2}\right)$

↖ kinetic energy of incoming particle

$$\Rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{q_1 q_2}{16\pi E \sin^2\left(\frac{\theta}{2}\right)} \right)^2$$

$$\Rightarrow \sigma = 2\pi \left(\frac{q_1 q_2}{16\pi E} \right)^2 \underbrace{\int_0^{\pi} \frac{\sin\theta \, d\theta}{\sin^4\left(\frac{\theta}{2}\right)}}_{\sim \text{ for } \theta \to 0 : \int \frac{d\theta}{\theta^3}} \longrightarrow \text{not finite !}$$

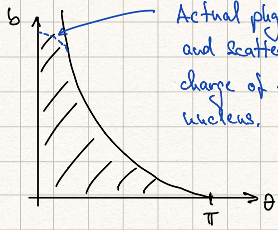
small angle divergence!



$b \to \infty$ for $\theta \to 0$
(potential leads to strong scattering even for $b \to \infty$)
↳ contradicts finite range assumption $r_0 \ll \rho_{max}$

Divergence due to the fact that the Coulomb potential $V(r) \sim \frac{1}{r}$ has "infinite range". ⇝ strongest possible large-r behavior of any potential related to a conservative force.

Note: This is not a physical problem because when $b \to \infty$ the potential of the whole atom needs to be considered, which is electrically neutral.
This is due to the fact that the whole electric charge inside a sphere with radius b around the scattering center needs to be considered.
So, Rutherford scattering formula represents an idealization that in practice is only valid for large scattering angles (which is exactly the correct limit to draw conclusions about the inner structure of the atom.



Actual physical relation of impact parameter and scattering angle due to the electric charge of the electron charges around the nucleus.

2.3. Elastic Scattering of a Spinless Particle off a Time-Independent Potential

In quantum theory the classic notion of the cross section cannot be used because there is no direct correspondence between the area segment $d\sigma$ some incoming particle enters and the solid angle segment $d\Omega(\theta,\phi)$ in which the scattered particle is detected.

↳ Differential cross section: (# = "number")

$$\frac{d\sigma}{d\Omega}(\theta,\phi) = \frac{\text{\# of particles that are scattered into the solid angle segment } d\Omega(\theta,\phi) \text{ per unit time devided by } d\Omega(\theta,\phi)}{\text{\# of incoming particles per unit time per area } (\perp \text{ to } \vec{k}_i)}$$

← "flux"

↳ Total cross section:

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{\text{\# of particles per unit time that are scattered at all}}{\text{\# of incoming particles per unit time per area } (\perp \text{ to } \vec{k}_i)}$$

= effective area the target represents to the incoming beam

These definitions are more general and work in classic as well as in quantum physics. They lead to same prescriptions used in Chap. 2.2.

General considerations: (Schrödinger picture)

$$H = T + V = \frac{\vec{p}^2}{2\mu} + V(\vec{x}) = -\frac{\vec{\nabla}^2}{2\mu} + V(\vec{x})$$

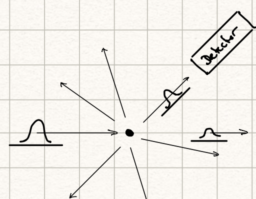
fct peaked at $\vec{k}_i$ in mom space

eigenfct of H with energy $E_{\vec{k}}$

↳ Solution is of the wave packet kind: $\psi_{\vec{k}_i}(\vec{x},t) = \int d^3\vec{k}\, A_{\vec{k}_i}(\vec{k})\, e^{-iE_{\vec{k}}t}\, \psi_{\vec{k}}(\vec{x})$

approximation used → $\approx e^{-iE_{\vec{k}_i}t}\, \psi_{\vec{k}_i}(\vec{x})$

forces us into argumentation tricks since $|\vec{r}| \gg S_{max}$ is strictly speaking unvalid



We request on $\psi_{\vec{k}_i}(\vec{x},t)$ that it describes:

(a) incoming and transmitted wave (e.g. in z-direction)
(b) scattered radially outgoing wave

We consider a stationary endless flux of incoming particles → we drop time-dependence (e^{-iEt}) (like bound state calculation)

↳ $\boxed{\text{Ausatz: } \psi_{\vec{k}_i}(\vec{x}) = N\left(e^{ik_i z} + \psi^{sc}_{\vec{k}_f}(\vec{x})\right), \quad |\vec{k}_i| = |\vec{k}_f|}$ "stationary scattering solution"

N: norm; $e^{ik_i z}$: incoming; $\psi^{sc}_{\vec{k}_f}$: outgoing scattered; $\underbrace{\text{incoming} \quad \text{outgoing scattered}}_{\text{transmitted (at } \theta = 0)}$

↳ We can learn about the $r\to\infty$ behavior of $\psi^{sc}_{\vec{k}_f}(\vec{x})$ assuming that $V(r)$ has only a finite range. More precise: $V(r>r_0)=0$ or $rV(r)\xrightarrow{r\to\infty}0$

For $r\to\infty$ (i.e. $r\gg S_{max}\gg r_0$) : $\left(\frac{\vec{\nabla}^2}{2\mu}+\frac{\vec{k}_i^2}{2\mu}\right)\psi_{\vec{k}_i}(\vec{x})=0$, also: $\left(\frac{\vec{\nabla}^2}{2\mu}+\frac{\vec{k}_i^2}{2\mu}\right)e^{ik_iz}=0$

$$\Rightarrow \left(\frac{\vec{\nabla}^2}{2\mu}+\frac{\vec{k}_i^2}{2\mu}\right)\psi^{sc}_{\vec{k}_f}(\vec{x})=0$$

Recall from QM 1: $\vec{\nabla}^2=-\vec{p}^2=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\vec{L}^2 \Rightarrow$ Separation of r and (θ,ϕ) dependence

↳ $\psi^{sc}_{k}(r,\theta,\phi)=\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\left(A_l\, \underbrace{j_l(kr)}_{\text{spherical Bessel fct}}+B_l\, \underbrace{n_l(kr)}_{\text{spherical Neumann fct}}\right)Y^m_l(\theta,\phi)$ ← spherical harmonic fcts

← See e.g. Schwabl I, Ch. 17

$$j_l(kr)\xrightarrow{r\to\infty}\frac{\sin(kr-l\pi/2)}{kr}$$
$$n_l(kr)\xrightarrow{r\to\infty}-\frac{\cos(kr-l\pi/2)}{kr}$$

We want an radially outgoing wave $\sim\frac{e^{ikr}}{r}$
(in analogy to e^{ikz} being a wave moving in pos. z dir.)
↳ $A_l=-iB_l$

The scattering wave fct has the general form:

$$\boxed{\psi^{sc}_{k}(r,\theta,\phi)\xrightarrow{r\to\infty}\frac{e^{ikr}}{r}\,f(E_k,\theta,\phi)}$$

"Scattering amplitude":
Since detectors always have a macroscopic distance to the target (i.e. $r\to\infty$ good approximation), $f(\theta,\phi)$ contains all information that is experimentally accessible

↳ Derivation of the differential cross section:

We use the scale hierarchy $r\gg S_{max}$ to argue that at the detector(s) only the radially outgoing wave is non-zero.
At the source of the beam we can likewise argue that only the incoming wave is non-zero.

Probability current of incoming wave:
(at the source of the beam)

$$\vec{j}_{in}\overset{QM1}{=}-\frac{i}{2\mu}\left[\psi^*_{in}(\vec{x})\vec{\nabla}\psi_{in}(\vec{x})-\psi_{in}(\vec{x})\vec{\nabla}\psi^*_{in}(\vec{x})\right] \qquad \psi_{in}(\vec{x})=Ne^{ikz}$$
$$=\mathrm{Re}\left[-i\frac{|N|^2}{\mu}e^{-ik_iz}(ik_i\vec{n}_z)e^{ik_iz}\right]=\frac{|N|^2}{\mu}k_i\vec{n}_z$$
$$=\underbrace{|N|^2}_{\text{\# of particles per unit volume in the incoming beam}}\;\underbrace{\vec{v}_{in}}_{\text{velocity of particles in the beam}}\quad\}\longrightarrow \text{flux of the beam}$$

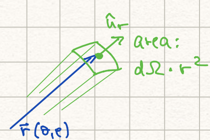
$|\vec{n}_i|^2=1$, $\vec{n}_i\cdot\vec{n}_j=\delta_{ij}$

Probability current of scattered wave:
(at the detector, $r\to\infty$ (!))

$$\vec{\nabla}=\vec{n}_r\frac{\partial}{\partial r}+\vec{n}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}+\vec{n}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$ ← only radial direction contributes for $r\to\infty$

$$\vec{j}_{sc}\overset{r\to\infty}{=}\frac{1}{\mu}|N|^2|f(\theta,\phi)|^2\,\mathrm{Re}\left[-i\frac{e^{-ik_fr}}{r}\left(ik_f\frac{e^{ik_fr}}{r}-\frac{e^{ik_fr}}{r^2}\right)\right]\vec{n}_r$$
$$\xrightarrow{r\to\infty}|N|^2\frac{|f(\theta,\phi)|^2}{r^2}\frac{k_f}{\mu}\vec{n}_r \qquad \left|\frac{k_f}{\mu}\right|=|\vec{v}_{in}| \quad \text{(elastic scattering)}$$

Outgoing flux entering solid angle $d\Omega(\theta,\phi)$:



$$\vec{j}_{sc}\cdot\vec{n}_r\cdot(r^2d\Omega)=|N|^2|f(\theta,\phi)|^2\,|\vec{v}_{in}|\,d\Omega(\theta,\phi)$$

Incoming flux in beam direction: $\vec{j}_{in} \cdot \vec{n}_z = |N|^2 |\vec{v}_{in}|$

$$\Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega}(\theta, \phi) = |f(E_i, \theta, \phi)|^2}$$

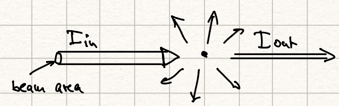
Comments:

- For $V = V(r)$ we have $f = f(E_i, \theta)$ (no ϕ-dependence)
- Common unit for cross sections: $1\,\text{barn} = 1\,b = (10^{-14}\,m)^2 = (0.02\,GeV)^{-2}$

  Total cross section for pp collisions at the LHC: $\sigma_{tot}^{LHC} \approx 0.1\,b \approx (3 \cdot 10^{-15}\,m)^2$
  ↳ Compare to nuclear radius $r_{nucleon} = 10^{-15}\,m$ (consistent)

- The total cross section at the LHC contains many different reaction channels (elastic and many inelastic). For one single channel the rule of thumb for the typical size of the total cross section is: $\sigma_{tot} \sim \frac{(\text{interaction strength})}{(\text{energy of the collision})^2}$

- Alternative interpretation of σ_{tot}: Due to the scattering, the total cross section, that the target represents for the incoming beam, can also be seen as the cause for a reduction of the intensity of the incoming beam (i.e. $I_{out} < I_{in}$):



$$\sigma_{tot} = \frac{(I_{in} - I_{out}) \cdot (\text{beam area})}{I_{in}}$$

$$\Leftrightarrow \quad I_{in} - I_{out} = I_{in} \underbrace{\frac{\sigma_{tot}}{\text{beam area}}}$$

fraction of total cross section to area of the beam.

It is assumed that the beam intensity is uniform over the whole beam area.

I: absolute particle intensity defined as # of particles delivered by beam per unit time

This connection is the background of the fundamental concept of probability conservation ($\approx$ particle # conservation in non-rel. quantum mechanics) in quantum theory which is coming from the Hermiticity
→ see Chap. 2.4.

2.4. The Optical Theorem

Stationary scattering solution : $\psi_{\vec{k}}(\vec{x}) \overset{r \gg r_0}{=} N\Big(\overset{\text{incoming}}{e^{ikz}} + \overset{\text{scattered}}{\frac{e^{ikr}}{r} f(E_k,\theta,\phi)}\Big)$

↳ For the determination of $\frac{d\sigma}{d\Omega}$ we have neglected the interference between the incoming and the scattered wave using that $r \gg s_{max}$.

But the interference term plays an important role in the global probability flow balance of the scattering process:

only direction $\hat{u}_r$ is relevant for $r \to \infty$ — subleading

$$\vec{j}_{total} = \mathrm{Re}\left[\psi_{\vec{k}}^*(\vec{x}) \frac{\vec{\nabla}}{i\mu} \psi_{\vec{k}}(\vec{x})\right] = \vec{j}_{in} + \vec{j}_{out} + \vec{j}_{interference}$$

$$= \frac{|N|^2}{\mu} \mathrm{Re}\left[-i\left(e^{-ikz} + f^* \frac{e^{-ikr}}{r}\right)\left(ik\,\vec{u}_z e^{ikz} + ikf \frac{e^{ikr}}{r} \vec{u}_r - \cancel{\frac{f}{r^2} e^{ikr} \vec{u}_r}\right)\right]$$

$$= \frac{|N|^2}{\mu} \mathrm{Re}\left[k\,\hat{u}_z + \frac{|f|^2}{r^2} k\,\hat{u}_r + \frac{f}{r} k\, e^{ik(r-z)} \hat{u}_r + \frac{f^*}{r} k\, e^{-ik(r-z)} \vec{u}_z\right]$$

$$= |\vec{j}_{in}|\,\vec{u}_z + \underbrace{|\vec{j}_{sc}|}_{= |\vec{j}_{in}| \frac{|f|^2}{r^2}} \vec{u}_r + \underbrace{|\vec{j}_{in}|\, \mathrm{Re}\left[\frac{f}{r} e^{ik(r-z)}\right] (\vec{u}_r + \vec{u}_z)}$$

Due to our argument that $s_{max} \ll r$ we conclude that the interference term is only relevant within the beam, i.e. for $\theta = 0$ ($\vec{u}_r = \vec{u}_z$, transmitted, $r = z$)
or $\theta = \pi$ ($\vec{u}_r = -\vec{u}_z$, back-reflected) ← $\hat{u}_r + \hat{u}_z = 0$
$\Rightarrow f(\theta = \pi) = 0$

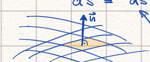
↳ Alternative derivation of the total cross section:

H Hermitian, $U(t,t_0) = e^{-iH(t-t_0)}$ unitary — see QM 1 Chap. 2.10.

$\Rightarrow$ continuity equation: $\frac{\partial}{\partial t} \rho(\vec{x},t) + \vec{\nabla} \vec{j}_{total}(\vec{x},t) = 0$, $\rho(\vec{x},t) = |\psi_{\vec{k}}(\vec{x},t)|^2$

We have $\int_{\mathbb{R}^3} d^3\vec{x}\, \rho(\vec{x},t) = \text{const} \Rightarrow \int_{\mathbb{R}^3} d^3\vec{x} \frac{\partial}{\partial t} \rho(\vec{x},t) = \frac{\partial}{\partial t} \int_{\mathbb{R}^3} d^3\vec{x}\, \rho(\vec{x},t) = 0$

$d\vec{s} = ds \cdot \vec{n}$ ← points outward w.r. to volume; ds: size of surface element



$$\Rightarrow \int_{\mathbb{R}^3} d^3\vec{x}\, \vec{\nabla} \vec{j}_{total}(\vec{x},t) \overset{\uparrow}{=} \lim_{r \to \infty} \int_{\substack{\text{surface} \\ \text{of sphere with} \\ \text{radius } r \text{ around target}}} d\vec{s}\, \vec{j}_{total}(\vec{x},t)$$

Gauß divergence theorem

$$= \lim_{r \to \infty} \int_{\partial V} d\vec{s}\, (\vec{j}_{in} + \vec{j}_{sc} + \vec{j}_{inter}) = 0$$

We calculate the three terms separately: $d\vec{s} = \vec{n}_r r^2 d\Omega$

$$\int_{\partial V} d\vec{s}\, \vec{j}_{in} = |\vec{j}_{in}| \int_{\partial V} d\vec{s}\, \vec{u}_z = |\vec{j}_{in}| \int d\Omega\, r^2 \overbrace{\vec{u}_r \cdot \vec{u}_z}^{\cos\theta} = |\vec{j}_{in}|\, r^2 \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta\, \cos\theta = 0$$

$$\int_{\partial V} d\vec{s}\, \vec{j}_{sc} = |\vec{j}_{in}| \int d\Omega\, r^2 \frac{|f|^2}{r^2} \overbrace{\vec{u}_r \cdot \vec{u}_r}^{=1} = |\vec{j}_{in}| \int d\Omega\, |f(E_k,\theta,\phi)|^2 = |\vec{j}_{in}|\, \sigma_{tot}$$

$$\int_{\partial V} d\vec{s}\, \vec{j}_{intr} = |\vec{j}_{in}| \int d\Omega\, r^2\, \mathrm{Re}\left[\frac{f}{r}\, e^{ik(r-z)}\right] (\vec{u}_r + \vec{u}_z)\cdot\vec{u}_r$$

$$= |\vec{j}_{in}|\, r \int d\Omega\, \mathrm{Re}\left[f(E_k,\theta,\phi)\, e^{ikr(1-\cos\theta)}\right](1+\cos\theta)$$

For $r \to \infty$ $e^{ikr(1-\cos\theta)}$ is strongly oscillating for $\cos\theta \neq 1$.
$\Rightarrow$ Only $\cos\theta = 1 \Leftrightarrow \theta = 0$ gives a finite contribution.

$$\xrightarrow{r\to\infty} |\vec{j}_{in}|\, 2\pi r\, \mathrm{Re}\left[f(E_k,\theta=0,\phi) \underbrace{\int_{-1}^{1} d\cos\, e^{ikr(1-\cos)}(1+\cos)}_{=\frac{1}{k^2r^2}(1-e^{2ikr}) + \frac{2i}{kr}}\right]$$

$$\xrightarrow{r\to\infty} |\vec{j}_{in}|\, \frac{4\pi}{k}\, \mathrm{Re}\left[i f(E_k,\theta=0,\phi)\right]$$

$$= -|\vec{j}_{in}|\, \frac{4\pi}{k}\, \mathrm{Im}\left[f(E_k,\theta=0,\phi)\right]$$

$\Rightarrow$ The optical theorem: $\boxed{\sigma_{tot} = \frac{4\pi}{k}\, \mathrm{Im}\left[f(E_k+i\epsilon,\theta=0,\phi)\right]}$

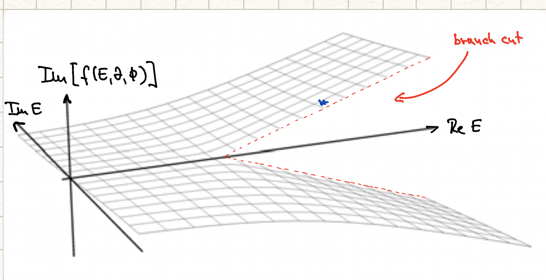
"The total cross section is proportional to the imaginary (absorptive) part of the forward ($\theta=0$) scattering amplitude."

Comments:

- The optical theorem is also true if inelastic processes take place in the scattering ($\rightarrow$ unitarity of time evolution becomes the fundamental property related to probability conservation.)

- The optical theorem implies that $f(E,\theta,\phi)$ is an analytic function in the energy E. In physics the analyticity of functions is related to their property that they are unambiguously defined. Their unambiguous character is related to causality.
  For the scattering amplitude $f(E,\theta,\phi)$ causality was implemented by the requirement that it had to describe an outgoing wave.

- The optical theorem implies that $f(E+i\epsilon,\theta=0,\phi)$ has a branch cut concerning its imaginary part along the real E-axis for all those energies where scattering can take place.



- One can reconstruct $f(E, \theta=0)$ for all complex E values, if $\sigma_{tot}(E)$ is known for all energies when scattering takes place.

$\sigma_{tot}(E) \to \mathrm{Im}[f(E, \theta=0, \phi)]$

↳ dispersion relation: $f(E) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dE' \, \mathrm{Im}[f(E')]}{E'-E-i\epsilon}$ $\epsilon > 0$ and infinitesimal

$$\mathrm{Re}[f(E)] = \frac{1}{\pi} \underset{\substack{\uparrow \\ \text{principal value}}}{P} \int_{-\infty}^{\infty} \frac{dE' \, \mathrm{Im}[f(E')]}{E'-E}$$

⟶ more on this later

2.5. The Green's Function Method

⟶ now: concrete solution for scattering amplitude f

Advantages:
- boundary conditions (e.g. causality) easy to implement
  ↳ analytic functions
- universal applicability
  → relativistic quantum field theory
  → multi-particle systems
  → numerical and analytical solutions
- particularly suited for perturbation theory ⟶ "Feynman rules"

Schrödinger equation for the stationary scattering solution:

$$\left(-\frac{\vec{\nabla}^2}{2\mu} + V(\vec{x}) - \frac{k^2}{2\mu}\right)\Psi_{\vec{k}}(\vec{x}) = 0 \quad , \quad E_k = \frac{k^2}{2\mu}$$

There are many different conventions concerning signs and factor of $\mathcal{O}(1)$ in text books.

$$\Leftrightarrow \quad D_k \Psi_{\vec{k}}(\vec{x}) = f(\vec{x}) \quad , \quad D_k := -\frac{1}{2\mu}(\underset{\substack{\uparrow \\ \text{acts on } \vec{x}!}}{\vec{\nabla}^2} + k^2) \quad , \quad f(\vec{x}) = -V(\vec{x})\Psi_{\vec{k}}(\vec{x})$$

General solution:

$$\Psi_{\vec{k}}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) + \Psi_{\vec{k}}(\vec{x})$$

$\phi_{\vec{k}}(\vec{x})$: $\frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}}$

$\Psi_{\vec{k}}(\vec{x})$ ⟵ a particular solution of $D_k \Psi_{\vec{k}} = f$

$\phi_{\vec{k}}(\vec{x})$: solution of homogeneous equation $D_k \phi_{\vec{k}} = 0$ (i.e. adapted such that boundary conditions are satisfied)

Formal determination of the particular solution:

↳ We assume that there exists a fct $G(\vec{x}, \vec{x}')$ ("Green's function") that satisfies

$$\boxed{D_k G_k(\vec{x}, \vec{x}') = \delta^{(3)}(\vec{x}-\vec{x}') \quad , \quad D_k = -\frac{1}{2\mu}(\vec{\nabla}^2 + k^2)}$$

"Green's function of the free Schrödinger equation"

Then $\Psi_{\vec{k}}(\vec{x}) = \int d^3\vec{x}' \, G_k(\vec{x}, \vec{x}') f(\vec{x}')$ is a particular solution

↳ Proof: $D_k \Psi_{\vec{k}}(\vec{x}) = D_k \int d^3\vec{x}' \, G_k(\vec{x}, \vec{x}') f(\vec{x}') = \int d^3\vec{x}' \, \delta(\vec{x}-\vec{x}') f(\vec{x}') = f(\vec{x})$ ⌞

→ Formal determination of the Green's function (still incomplete!)

$$-\frac{1}{2\mu}\left(\vec{\nabla}^2 + k^2\right) G_k(\vec{x},\vec{x}\,') = \delta^{(3)}(\vec{x}-\vec{x}\,')$$

Method A: → Set of all free solutions is complete: $\phi_{\vec{k}}(\vec{x}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} = \langle \vec{x}|\vec{k}\rangle$

$$\Rightarrow G_k(\vec{x},\vec{x}\,') = \int d^3k'\, \phi_{\vec{k}'}(\vec{x})\, c(k^2, k'^2, \vec{x}\,')$$ expand $\vec{x}$-dependence in $\phi_{\vec{k}}(\vec{x})$ eigenfunctions

We have $D_k \phi_{\vec{k}'}(\vec{x}) = -\frac{1}{2\mu}(k^2 - k'^2)\phi_{\vec{k}'}(\vec{x})$

$$\Rightarrow D_k G_k(\vec{x},\vec{x}\,') = \int d^3k' \left(-\frac{k^2-k'^2}{2\mu}\right)\phi_{\vec{k}'}(\vec{x})\, c(k^2,k'^2,\vec{x}\,') \stackrel{!}{=} \delta^{(3)}(\vec{x}-\vec{x}\,')$$

We have $\int d^3x\, \phi^*_{\vec{k}}(\vec{x})\phi_{\vec{k}}(\vec{x}) = \delta^{(3)}(\vec{k}-\vec{k}')$ orthonormality

$\int d^3k\, \phi_{\vec{k}}(\vec{x})\phi^*_{\vec{k}}(\vec{x}\,') = \delta^{(3)}(\vec{x}-\vec{x}\,')$ completeness

$$\Rightarrow c(k^2,k'^2,\vec{x}\,') = -\frac{2\mu}{k^2-k'^2}\phi^*_{\vec{k}'}(\vec{x}\,')$$

$$\Rightarrow G_k(\vec{x},\vec{x}\,') = 2\mu\int d^3k' \frac{\phi_{\vec{k}'}(\vec{x})\phi^*_{\vec{k}'}(\vec{x}\,')}{k'^2-k^2} = \int d^3k' \frac{\phi_{\vec{k}'}(\vec{x})\phi^*_{\vec{k}'}(\vec{x}\,')}{E_{\vec{k}'}-E_{\vec{k}}}$$ Configuration space Green's function

$$= \langle \vec{x}| \int d^3k' \frac{|\vec{k}'\rangle\langle\vec{k}'|}{E_{\vec{k}'}-E_{\vec{k}}}|\vec{x}\,'\rangle =: \langle\vec{x}|G_k|\vec{x}\,'\rangle$$

$$= 2\mu\int\frac{d^3k'}{(2\pi)^3}\frac{e^{i\vec{k}'(\vec{x}-\vec{x}\,')}}{\vec{k}'^2-\vec{k}^2} = \int\frac{d^3k'}{(2\pi)^3}\frac{e^{i\vec{k}'(\vec{x}-\vec{x}\,')}}{E_{\vec{k}'}-E_{\vec{k}}}$$

formal operator G_k: $D_k G_k = (H-E_{\vec{k}})G_k = \mathbb{1}$

Method B: → Momentum space Green's function

Free Schrödinger equation in mom space: $\left(\frac{\vec{p}^2}{2\mu}-\frac{\vec{k}^2}{2\mu}\right)\tilde{\psi}(\vec{p}) = 0$

$$\rightarrow \left(\frac{\vec{p}^2-\vec{k}^2}{2\mu}\right)\tilde{G}_k(\vec{p},\vec{p}\,') = (E_{\vec{p}}-E_{\vec{k}})\tilde{G}(\vec{p},\vec{p}\,') = \delta^{(3)}(\vec{p}-\vec{p}\,')$$ ← purely algebraic equation

$$\Rightarrow \tilde{G}_k(\vec{p},\vec{p}\,') = \frac{\delta^{(3)}(\vec{p}-\vec{p}\,')}{E_{\vec{p}}-E_{\vec{k}}} = 2\mu\frac{\delta^{(3)}(\vec{p}-\vec{p}\,')}{\vec{p}^2-\vec{k}^2} = \langle\vec{p}|G_k|\vec{p}\,'\rangle$$

Comments:

- Consistency between config and mom space Green's functions:

$$G_k(\vec{x},\vec{x}\,') = \langle\vec{x}|G_k|\vec{x}\,'\rangle = \int d^3p\, d^3p'\langle\vec{x}|\vec{p}\rangle\tilde{G}_k(\vec{p},\vec{p}\,')\langle\vec{p}\,'|\vec{x}\,'\rangle$$ $\langle\vec{x}|\vec{p}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\vec{p}\vec{x}}$

$$= \int\frac{d^3p}{(2\pi)^3}\int d^3p'\, e^{i(\vec{p}\vec{x}-\vec{p}\,'\vec{x}\,')}\frac{\delta^{(3)}(\vec{p}-\vec{p}\,')}{E_{\vec{p}}-E_{\vec{k}}} = \int\frac{d^3p}{(2\pi)^3}\frac{e^{i\vec{p}(\vec{x}-\vec{x}\,')}}{E_{\vec{p}}-E_{\vec{k}}}$$ agrees with (A) ✓

- We see that $G_k(\vec{x},\vec{x}\,') = G_k(\vec{x}-\vec{x}\,',0)$
- There is a serious problem in $G_k(\vec{x},\vec{x}\,')$ because of the singularity at $k^2 = k'^2$.

→ Computation of the Green's function

So far we only made formal manipulations. The singularity at $k^2 = k'^2$ in $G_k(\vec{x},\vec{x}')$ indicates, however, that the Green's function defined that way is not ambiguity-free and certainly not an analytic function in E_k

⇒ Something is missing!

We need to input more physics! "$+i\epsilon$-prescription"

Let's resolve the issue by shifting E_k infinitesimally into the upper complex half plane: $E_k \to E_k + i\epsilon$, $\epsilon > 0$ but infinitesimally small

- solution now ambiguity-free ✓
- solution is analytic (except at poles and/or cuts) ✓
- Why not using $E_k \to E_k - i\epsilon$ or something else? → See later. Let's calculate first.

⇒ $\frac{1}{2\mu} G_k(\vec{x},\vec{x}') = \frac{1}{2\mu} G_k(\vec{r},0)$ $\quad \vec{r} = \vec{x} - \vec{x}'$, $r = |\vec{r}|$

change of variables: $p \to -p$ (only here!!)

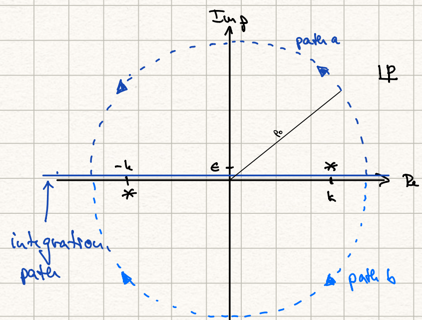
$$= \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\vec{p}\vec{r}}}{p^2-k^2-i\epsilon} = \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos \int_0^\infty \frac{p^2\,dp}{(2\pi)^3} \frac{e^{ipr\cos}}{p^2-k^2-i\epsilon} = 2\pi \int_0^\infty \frac{p^2\,dp}{(2\pi)^3} \frac{1}{p^2-k^2-i\epsilon} \frac{i}{pr}\left(e^{-ipr} - e^{ipr}\right)$$

$$= -\frac{2\pi i}{r(2\pi)^3} \int_{-\infty}^{+\infty} \frac{p\,dp}{p^2-k^2-i\epsilon} e^{ipr}$$

⇒ $$\frac{1}{p^2-k^2-i\epsilon} \overset{k>0}{=} \frac{1}{p^2-(k+i\epsilon)^2} = \frac{1}{(p-k-i\epsilon)(p+k+i\epsilon)}$$

$$= \frac{1}{2k+i\epsilon}\left(\frac{1}{p-k-i\epsilon} - \frac{1}{p+k+i\epsilon}\right)$$

→ Integrand has 2 poles at $p = \pm(k+i\epsilon)$



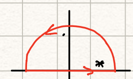
"Closing-the-Contour method"

The method is typically described in books as follows: "We need to close the contour in the upper complex p-plane, such that the closing contour does not contribute, and then pick up the pole inside the contour using the residue theorem."

Consider the p integral along path a in the upper complex plane: $p(\varphi) = p_0 e^{i\varphi}$, $dp = i p_0 e^{i\varphi} d\varphi$, $e^{i\varphi} = \cos\varphi + i\sin\varphi$

$$\int_{\text{path a}} \frac{p\,dp}{p^2-k^2} e^{ipr} = \int_0^\pi \underbrace{\frac{i p_0^2 e^{2i\varphi}}{p_0^2 e^{2i\varphi} - k^2}}_{\to\, i \text{ for } p_0\to\infty} e^{ip_0 r\cos\varphi}\, e^{-p_0 r \sin\varphi}\, d\varphi \xrightarrow{p_0\to\infty} 0$$

⇒ Path a does not contribute for $p_0 \to \infty$ because the e^{ipr} is suppressed in the upper complex p-half-plane.



So we can write: $$\int_{-\infty}^{+\infty} \frac{p\,dp}{p^2-k^2-i\epsilon} e^{ipr} = \lim_{p_0\to\infty} \left(\int_{-p_0}^{+p_0} + \int_{\text{path a}} \right) \underbrace{\frac{p}{p^2-k^2-i\epsilon} e^{ipr}}_{= f(p)} dp$$

We can now use the residue theorem: $$\oint_{\substack{\text{contour in}\\ \text{positive direction = counter clockwise !}}} f(z)\,dz = 2\pi i \sum (\text{residues of } f \text{ inside closed contour})$$

$$\mathrm{Res}_f(p=k+i\epsilon) = \lim_{p\to k+i\epsilon} (p-k-i\epsilon) f(p) = \lim_{p\to k+i\epsilon} \cancel{(p-k-i\epsilon)} \frac{p}{\cancel{(p-k-i\epsilon)}(p+k+i\epsilon)} e^{ipr} = \frac{1}{2} e^{i(k+i\epsilon)r}$$

can be neglected from now on.

$$\Rightarrow \int_{-\infty}^{+\infty} \frac{p\,dp}{p^2-k^2-i\epsilon} e^{ipr} = 2\pi i \frac{1}{2} e^{ikr} = i\pi e^{ikr}$$

<u>Note:</u> Path b in the lower complex half-plane leads to a divergent integrand ($\sim e^{+\text{Por fixe}}$) and is useless for the method in this case. However, there are calculations where that path is the correct one. You have to check case by case.

$$\boxed{G_k^{(+)}(\vec{x},\vec{x}') = \frac{\mu}{2\pi} \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}}$$

"retarded Green's function"

→ The prescription $E_k \to E_k + i\epsilon$ is related to an <u>outgoing wave</u> and the Green's function with the correct boundary condition and causality structure needed for the scattering problem.

collision is the cause for the outgoing wave

If we use the prescription $E_k \to E_k - i\epsilon$ ("$-i\epsilon$ prescription") the result for the Green's function has the form
$$G_k^{(-)}(\vec{x},\vec{x}') = \frac{\mu}{2\pi} \frac{e^{-ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \qquad (\text{"advanced Green's function"})$$

This is related to an incoming wave and not the proper Green's function we need to use for the scattering problem. It does not have the correct causality structure for the problem.

<u>But:</u> $G_k^{(-)}$ is also a mathematically (formally) correct Green's function for the free Schrödinger equation.

These are general principles!

→ <u>Causality</u> tells us, which of the mathematically possible Green's functions is the one we need to use.

→ After imposing causality the Green's function is <u>unique and unambiguous</u> and we are dealing with <u>analytic functions.</u>

<u>Complete formulae for the retarded Green's function:</u>

$$G_k = \int d^3\vec{p} \frac{|\vec{p}\rangle\langle\vec{p}|}{E_{\vec{p}} - E_{\vec{k}} - i\epsilon} = 2\mu \int d^3\vec{p} \frac{|\vec{p}\rangle\langle\vec{p}|}{\vec{p}^2 - \vec{k}^2 - i\epsilon}, \qquad (H - E_{\vec{k}}) G_k = \mathbb{1}$$

$$G_k(\vec{x},\vec{x}') = \langle\vec{x}|G_k|\vec{x}'\rangle = \int d^3\vec{p} \frac{\langle\vec{x}|\vec{p}\rangle\langle\vec{p}|\vec{x}'\rangle}{E_{\vec{p}} - E_{\vec{k}} - i\epsilon}, \qquad (H - E_{\vec{k}}) G_k(\vec{x},\vec{x}') = \delta^{(3)}(\vec{x}-\vec{x}')$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}}{E_{\vec{p}} - E_{\vec{k}} - i\epsilon} = 2\mu \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}}{\vec{p}^2 - \vec{k}^2 - i\epsilon}$$

$$\tilde{G}_k(\vec{p},\vec{p}') = \langle\vec{p}|G_k|\vec{p}'\rangle = \frac{\delta^{(3)}(\vec{p}-\vec{p}')}{E_{\vec{p}} - E_{\vec{k}} - i\epsilon} = 2\mu \frac{\delta^{(3)}(\vec{p}-\vec{p}')}{\vec{p}^2 - \vec{k}^2 - i\epsilon}, \qquad (H - E_{\vec{k}}) \tilde{G}_k(\vec{p},\vec{p}') = \delta^{(3)}(\vec{p}-\vec{p}')$$

General properties of the Green's function

- The different $i\varepsilon$ - prescriptions are only relevant if we want to consider the Green's function to determine solutions of the Schrödinger equation
  ⇒ $E_{\vec{k}} \in \mathbb{R}_+$

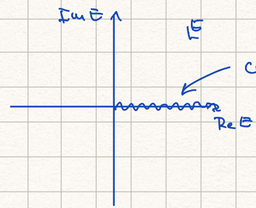
  Only then the ambiguity in its definition arises, because the eigenenergies $E_{\vec{p}}$ are $\in \mathbb{R}_+$ as well.

  But we can also consider the Green's function as an analytic function for complex energies. The result then reads:

$$G(E, \vec{x}, \vec{x}') = \frac{\mu}{2\pi} \frac{\exp\left(-\sqrt{-mE'}\,|\vec{x}-\vec{x}'|\right)}{|\vec{x}-\vec{x}'|}$$

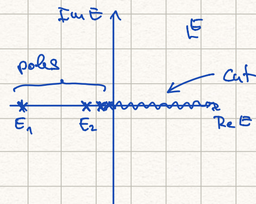
  $G(E, \vec{x}, \vec{x}')$ is analytic except $E \in$ spectrum of H = set of eigenenergies
  - G has branch cuts where the spectrum is continuous
  - G has poles at discrete eigenenergies

Green's fct for $H = \frac{\vec{p}^2}{2\mu}$: spectrum $= \mathbb{R}_{+,0}$



(see picture on page 03/18/2018 5)

Green's fct for $H = \frac{\vec{p}^2}{2\mu} - \frac{1}{4\pi}\frac{e^2}{|\vec{x}|}$ (Coulomb problem): spectrum $= \mathbb{R}_{+,0} \cup \left\{ E_n = -\frac{\mu e^4}{2n^2},\ n \in \mathbb{N} \right\}$



⇒ The Green's function (as a function in the complex E plane) contains all information about the solutions of the system defined by the Hamilton operator H and it is also the basis for perturbation theory to account for additional effects.

→ Determination of the scattering amplitude

We can now write down the physically correct solution for the stationary scattering problem:

$$\boxed{\psi_{k_i}(\vec{x}) = N e^{i\vec{k}_i\vec{x}} + \int d^3\vec{x}'\, G^{(+)}_{k_i}(\vec{x},\vec{x}')\left(-V(\vec{x}')\right)\psi_{\vec{k}_i}(\vec{x})}$$

$$G^{(+)}_{k}(\vec{x},\vec{x}') = \frac{\mu}{2\pi}\frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}, \quad k=|k_i|$$

$\vec{k}_i$: incoming particle momentum

To get the expression for the scattering amplitude $f(E,\theta,\phi)$
we still have to expand for $r=|\vec{x}| \to \infty$: $r \gg r'=|\vec{x}'|$ because V has finite range $r_0 \ll r$

unit vector in r-direction

$$|\vec{x}-\vec{x}'| = \sqrt{r^2 - 2\vec{x}\vec{x}' + r'^2} \xrightarrow{r\to\infty} r\sqrt{1-2\frac{\vec{x}\vec{x}'}{r^2}+\frac{r'^2}{r^2}} \approx r\left(1-\frac{\vec{x}\vec{x}'}{r^2}\right) \approx r - \frac{\vec{x}}{r}\vec{x}' = r - \vec{u}_r\vec{x}'$$

$$\Rightarrow \frac{\mu}{2\pi}\frac{e^{ik_i|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \xrightarrow{r\to\infty} \frac{\mu}{2\pi}\frac{e^{ik_i r}}{r}e^{-ik_i\vec{u}_r\vec{x}'}, \quad k_i\vec{u}_r = \vec{k}_f \quad (|\vec{k}_i| = |\vec{k}_f|)$$

$$\hookrightarrow \quad \psi_{k_i}(\vec{x}) \overset{r\to\infty}{=} N e^{i\vec{k}_i\vec{x}} + \frac{e^{ik_i r}}{r}\frac{\mu}{2\pi}\int d^3\vec{x}'\, e^{-i\vec{k}_f\vec{x}'}\left(-V(\vec{x}')\right)\psi_{\vec{k}_i}(\vec{x}') \qquad |\vec{k}_i| = |\vec{k}_f|$$

$$\boxed{f(E_{k_i},\theta,\phi) = -\frac{\mu}{2\pi N}\int d^3\vec{x}\; e^{-i\vec{k}_f\vec{x}}\, V(\vec{x})\,\psi_{\vec{k}_i}(\vec{x})} \longrightarrow \text{not an explicit solution}$$

→ To get an explicit (approximate) solution we use the assumption that the scattering overall is a very small effect: $\Rightarrow \psi_{\vec{k}_i}(\vec{x}) = N e^{i\vec{k}_i\vec{x}} + \underbrace{O(V)}_{\text{small correction}}$

$$\hookrightarrow \boxed{f(E_{k_i},\theta,\phi) \approx -\frac{\mu}{2\pi}\int d^3\vec{x}\; e^{-i\overbrace{(\vec{k}_f-\vec{k}_i)}^{\text{"momentum transfer"}}\vec{x}}\, V(\vec{x})} \qquad \text{"Born approximation"}$$

→ In the Born approximation the scattering amplitude is proportional to the Fourier transform of the config space potential w.r. to the "momentum transfer" $\vec{k}_f - \vec{k}_i$ (= momentum that the scattering center is giving to the scattered particle)

→ The Born approximation may be already a good approximation of the exact result. However sometimes more precision is needed.

2.6. Neumann Perturbation Series

→ Approach to carry out time-independent perturbation theory for continuous states.

→ Assumption: $\boxed{e^{i\vec{k}\vec{x}} \gg \int d^3\vec{x}'\, G(\vec{x},\vec{x}')\, V(\vec{x}')\, \psi_k(\vec{x}) \quad \Rightarrow \text{ We expand in powers of } V.}$ → Must be true for $|\vec{x}'| \leq r_0$ (range of potential)

$\left(G_k \equiv G_k^+ \text{ from now on} \right)$

Perturbative expansion for the time-independent scattering solution:

We set norm $N = \frac{1}{(2\pi)^{3/2}}$

<u>0th approx.:</u> $\psi_{\vec{k}}^{(0)}(\vec{x}) = \phi_{\vec{k}}(\vec{x}) = \frac{e^{i\vec{k}\vec{x}}}{(2\pi)^{3/2}} = \langle \vec{x} | \vec{k} \rangle$

<u>1st approx.:</u> (Born approximation)

$$\psi_{\vec{k}}^{1st}(\vec{x}) = \psi_{\vec{k}}^{(0)}(\vec{x}) + \psi_{\vec{k}}^{(1)}(\vec{x})$$

$$= \phi_{\vec{k}}(\vec{x}) + \int d^3\vec{x}'\, G_k(\vec{x},\vec{x}')\,(-V(\vec{x}'))\,\phi_k(\vec{x}) = \langle \vec{x} | [1 - G_k V] | \vec{k} \rangle$$

<u>2nd approx.:</u> $\psi_{\vec{k}}^{2nd}(\vec{x}) = \psi_{\vec{k}}^{1st}(\vec{x}) + \int d^3\vec{x}'\, d^3\vec{x}''\, G_k(\vec{x},\vec{x}')\,(-V(\vec{x}'))\,G_k(\vec{x}',\vec{x}'')\,(-V(\vec{x}''))\,\phi_k(\vec{x}'')$

⋮

$$= \langle \vec{x} | [1 - G_k V + G_k V G_k V] | \vec{k} \rangle$$

<u>All order solution:</u> (formal) $\psi_{\vec{k}}(\vec{x}) = \langle \vec{x} | [1 - G_k V + G_k V G_k V - G_k V G_k V G_k V + \ldots] | \vec{k} \rangle$

$$= \langle \vec{x} | \frac{1}{1 + G_k V} | \vec{k} \rangle$$

Perturbative expansion for the scattering amplitude:

<u>1st approx.:</u> (Born approximation)

$$f^{1st}(E_{k_i}, \theta, \phi) = \frac{\mu}{2\pi} \int d^3\vec{x}\, e^{-i\vec{k}_f\vec{x}}\,(-V(\vec{x}))\, e^{+i\vec{k}_i\vec{x}}$$

$$= 4\pi^2\mu \int d^3\vec{x}\, \phi^*_{\vec{k}_f}(\vec{x})\,(-V(\vec{x}))\,\phi_{\vec{k}_i}(\vec{x})$$

$$= -4\pi^2\mu\, \tilde{V}(\vec{k}_f, \vec{k}_i)$$

$$= 4\pi^2\mu\, \underbrace{\langle \vec{k}_f | -V | \vec{k}_i \rangle}$$

→ "Born T matrix element"

↑

"transition"

All order Solution: (formal) $k = |\vec{k}_i| = |\vec{k}_f|$ "T matrix element"

$$f^{1st}(E_{k_i},\theta,\phi) = 4\pi^2\mu \underbrace{\langle \vec{k}_f | -V \frac{1}{1+G_k V} | \vec{k}_i \rangle}_{\text{"T matrix element"}}$$

$$= 4\pi^2\mu \langle \vec{k}_f | -V + V G_k V - V G_k V G_k V + \dots | \vec{k}_i \rangle \qquad k^2 = \vec{k}_i^2 = \vec{k}_f^2$$

$$= 4\pi^2\mu \Big\{ -\tilde{V}(\vec{k}_f,\vec{k}_i) + \int d^3\vec{q}\, \tilde{V}(\vec{k}_f,\vec{q}) \frac{2\mu}{\vec{q}^2 - k^2 - i\epsilon} \tilde{V}(\vec{q},\vec{k}_i) - \dots$$

$$\dots + (-1)^{n+1} \int d^3\vec{q}_1 \dots d^3\vec{q}_n\, \tilde{V}(\vec{k}_f,\vec{q}_1) \frac{2\mu}{\vec{q}_1^2 - k^2 - i\epsilon} \tilde{V}(\vec{q}_1,\vec{q}_2) \dots \frac{2\mu}{\vec{q}_n^2 - k^2 - i\epsilon} \tilde{V}(\vec{q}_n,\vec{k}_i) + \dots \Big\}$$

Feynman Rules for the T matrix element in Momentum Space

→ graphical notation for the analytic expressions, which – however – intuitively illustrate the actual physical processes that take place.

→ Comment: Name "Feynman rules" comes historically from relativistic quantum field theory, where they are essential for doing computations due to complexity. Here the advantage of Feynman rules is not so obvious.

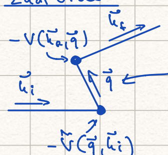
Born approximation

interaction factor $-\tilde{V}(\vec{k}_f,\vec{k}_i)$ for transition $|\vec{k}_i\rangle \longrightarrow |\vec{k}_f\rangle$

$\Longrightarrow$ $\boxed{-\tilde{V}(\vec{k}_f,\vec{k}_i)}$

related to classical limit

2nd order

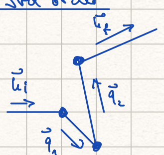


intermediate propagation factor of particle without interaction: $2\mu/(\vec{q}^2 - \vec{k}_i^2 - i\epsilon)$ ⊕ sum over all $\vec{q}$

$\Longrightarrow$ $\boxed{\int d^3\vec{q} \left(-\tilde{V}(\vec{k}_f,\vec{q})\right) \frac{2\mu}{\vec{q}^2 - \vec{k}_i^2 - i\epsilon} \left(-\tilde{V}(\vec{q},\vec{k}_i)\right)}$

Particle has the "virtual" momentum $\vec{q}$. Describes a pure quantum effect beyond the classic level: "virtual particle"

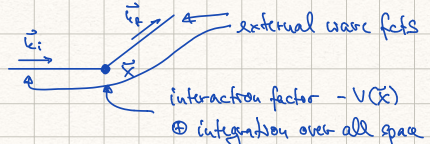
3rd order



. . . .

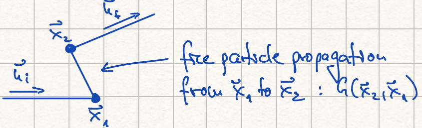
Feynman Rules for the T matrix element in Configuration Space

Born approximation



$$\Longrightarrow \quad \boxed{\int d^3\vec{x}\; \frac{e^{-i\vec{k}_f\vec{x}}}{(2\pi)^{3/2}} \left(-V(\vec{x})\right) \frac{e^{i\vec{k}_i\vec{x}}}{(2\pi)^{3/2}}}$$

2nd order



$$\Longrightarrow \quad \boxed{\int d^3\vec{x}_1\, d^3\vec{x}_2\; \frac{e^{-i\vec{k}_f\vec{x}_2}}{(2\pi)^{3/2}} \left(-V(\vec{x}_2)\right) G_{k_i}(\vec{x}_2,\vec{x}_1) \left(-V(\vec{x}_1)\right) \frac{e^{i\vec{k}_i\vec{x}_1}}{(2\pi)^{3/2}}}$$

⋮

When is the Neumann series a good expansion?

→ We carry out a number of qualitative considerations.

- We already see from formulae: Series appears sign-alternating for $V(\vec{x}) > 0$.
  ↳ Convergence better for repulsive potential.

- We now analyze a bit more:

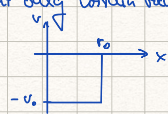
$$\psi_{\vec{k}}(\vec{x}) \sim e^{i\vec{k}\vec{x}} + \psi^{sc}(\vec{x}) \;:\; \rightsquigarrow\; e^{i\vec{k}\vec{x}} \overset{!}{\gg} \psi^{sc}(\vec{x}) \quad \text{for } |\vec{x}| \lesssim r_0 \quad \text{(range of potential)}$$

↳ consider $\vec{x}=0$ (at centre of potential) : we have $e^{i\vec{k}\vec{x}} = 1$ ⤳ we want: $|\psi^{sc}(0)| \ll 1$

$$|\psi^{sc}(\vec{x}=0)| \overset{\text{Born}}{=} \left|\frac{\mu}{2\pi}\int d^3\vec{x}'\, \frac{e^{ikx'}}{x'} V(\vec{x}') e^{i\vec{k}\vec{x}'}\right| = \frac{2\mu}{k}\left|\int_0^\infty dr\, e^{ikr} \sin(kr)\, V(r)\right|$$

Case 1: low-energy scattering: $kx' \lesssim kr_0 \ll 1$ (relevant only within range of potential!)

$$|\psi^{sc}(0)| \sim \frac{2\mu}{k}\int_0^{r_0} dr\; kr\, V_0 = \mu r_0^2 V_0 \overset{!}{\ll} 1$$



↳ $V_0 \ll \dfrac{1}{\mu r_0^2}$

What does the inequality mean? → consider ground state (lowest energy bound state) of an attractive potential

average momentum $\sim \frac{1}{r_0}$ (= inverse size)
average kin. energy $\sim \left(\frac{1}{r_0}\right)^2/\mu \sim \frac{1}{\mu r_0^2}$

↳ $V_0 \ll \frac{1}{\mu r_0^2}$ means that V is too shallow to allow for a bound state

⟹ Convergence better if the potential does not have bound states, because – otherwise – these states can to additional non-trivial effects not properly treated by the Neumann series.

Case 2: high-energy scattering (but still non-relativistic)

$\leadsto$ $kr \gg 1$, $\sin kr = \frac{1}{2i}\left(e^{ikr} - e^{-ikr}\right)$

$$|\psi^{sc}(0)| = \frac{\mu}{k}\left|\int_0^\infty dr\,\left(e^{2ikr}-1\right)V(r)\right| \approx \frac{\mu}{k}\left|\int_0^\infty dr\, V(r)\right| \sim \frac{\mu}{k}V_0 r_0 \overset{!}{\ll} 1$$

$\uparrow$ oscillate strongly

$\frac{\mu V_0 r_0}{k} \ll 1$ can be always easily satisfied if only the energy $E_i = \frac{k_i^2}{2\mu}$ is high enough.

$\leadsto$ higher energy $\longrightarrow$ interaction time with potential smaller

Note: The Neumann series is in general not convergent – even if the conditions are satisfied and the first terms in the series look convergent. $\longrightarrow$ "asymptotic expansion"

2.7. Generalizations

Differential cross section for spinless particle off stationary scattering centre revisited

$\longrightarrow$ We rewrite our known formula to better see how to generalize it ($\leadsto$ time-dependent problems, multiparticle scattering, particles with spin, ...)

Differential elastic cross section for the scattering of a particle off the potential of an infinitely heavy particle:

$$\frac{d\sigma}{d\Omega} = |f(E_i,\theta,\phi)|^2 = (2\pi)^4\mu^2\left|\langle\vec{k}_f|-V\frac{1}{1+GV}|\vec{k}_i\rangle\right|^2$$

probability current of incoming beam : $|\vec{j}_{in}| = |\vec{v}_i|\frac{1}{(2\pi)^3} = \frac{k_i}{\mu}\frac{1}{(2\pi)^3}$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{1}{|\vec{j}_{in}|}\left|\langle\vec{k}_f|-V\frac{1}{1+GV}|\vec{k}_i\rangle\right|^2 (2\pi)k_i\mu$$

δ-fct expressing energy conservation: $\delta\left(\frac{\vec{k}_f^2}{2\mu} - \frac{\vec{k}_i^2}{2\mu}\right) = \delta\left(\frac{1}{2\mu}(k_f+k_i)(k_f-k_i)\right) = \frac{\mu}{k_i}\delta(k_f-k_i)$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{1}{|\vec{j}_{in}|}\int dk_f\, k_f^2\,\frac{\mu}{k_f}\delta(k_f-k_i)\left|\langle\vec{k}_f|-V\frac{1}{1+GV}|\vec{k}_i\rangle\right|^2(2\pi)$$

$$= \frac{1}{|\vec{j}_{in}|}\int dk_f\, k_f^2\left|\langle\vec{k}_f|-V\frac{1}{1+GV}|\vec{k}_i\rangle\right|^2(2\pi)\,\delta\left(\frac{\vec{k}_f^2}{2\mu}-\frac{\vec{k}_i^2}{2\mu}\right)$$

$\int dk\, k^2\, d\Omega = \int d^3\vec{k}$

$$\leadsto \boxed{d\sigma = \frac{1}{|\vec{j}_{in}|}\left|\langle\vec{k}_f|-V\frac{1}{1+GV}|\vec{k}_i\rangle\right|^2(2\pi)\,\delta(E_f-E_i)\,d^3\vec{k}_f}$$

normalization w.r.t. to incoming particle intensity

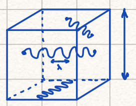
energy conservation for elastic scattering

final state phase space differential (for elastic scattering)

FOR MASSIVE FINAL STATE PARTICLES ?

→ Final state phase space: ⇝ We want to understand the counting of states more systematically.

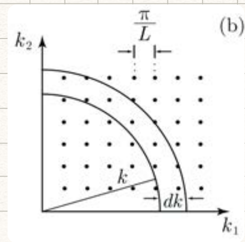
↳ Density of free particle states: Consider cube with side length L



$V = L^3 \to \infty$

Only integer multiples of $\frac{\lambda}{2}$ fit into the cube.
Possible momenta (wave vectors):
$\vec{k} = \frac{\pi}{L}(n_1, n_2, n_3)$, $n_i = 0, 1, 2, 3, \ldots$

Each vector (n_1, n_2, n_3) corresponds to one state.



Number of states for momenta in intervall $[k, k+\delta k]$: $\frac{1}{8}\frac{4\pi k^2 dk}{(\pi/L)^3} = \frac{V}{(2\pi)^3} 4\pi k^2 dk$

↳ Number of states associated to the momentum volume element $d^3\vec{k}$: $\frac{V}{(2\pi)^3} d^3\vec{k}$

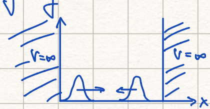
Norm of free particle states (in cube with $V = L^3$) : $\langle \vec{k} | \vec{k} \rangle = \int_V d^3\vec{x}\ \phi_k^*(\vec{x})\, \phi_k(\vec{x}) = \int_V \frac{d^3\vec{x}}{(2\pi)^3} = \frac{V}{(2\pi)^3}$

⇒ We see that $\frac{1}{\langle \vec{k}_f | \vec{k}_f \rangle} \frac{V}{(2\pi)^3} d^3\vec{k}_f = d^3\vec{k}_f$ sums over all possible final state states $|\vec{k}_f\rangle$ and also divides out their norm.
So using $|\vec{k}_f\rangle$ states as final states and $d^3\vec{k}_f$ for the final state integration correctly sums over normalized states.

↳ We now can generalize to multiparticle final states:

$$\boxed{|\langle in | \ldots | \vec{k}_f \rangle|^2 d^3\vec{k}_f \longrightarrow |\langle in | \ldots | \vec{k}_{f_1}, \ldots, \vec{k}_{f_n} \rangle|^2 d^3\vec{k}_{f_1} \ldots d^3\vec{k}_{f_n} \quad \text{for} \quad \begin{matrix} \langle \vec{x} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} \\ \langle \vec{k} | \vec{k}' \rangle = \delta^{(3)}(\vec{k}-\vec{k}') \end{matrix}}$$

Note: It appears that only positive momenta $k_i > 0$ fit inside the box and that we illegally generalized it to all momenta simply by reshuffling an overall factor 8.
But what we did is perfectly ok.
↳ We used the solutions of the problem "particle inside an impenetrable box" (see QM1 lecture) which can represent waves moving in positive ($k>0$) and in negative direction ($k<0$).
The way this works mathematically is that each solution can be rewritten in terms of free particle exponentials : e.g. $\sin(kx) = \frac{1}{2i}(e^{ikx} - e^{-ikx})$



↳ Alternative argumentation for the counting of states that fit in the box:

Think-Exercise !

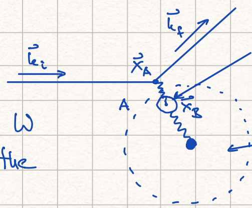
Use periodic boundary conditions : $\psi(\vec{x}) = \psi(\vec{x} \pm (L, L, L))$

⇒ Possible momenta (wave vectors): $\vec{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$ with $n_i = 0, \pm 1, \pm 2, \ldots$

Number of states for momenta in intervall $[k, k+\delta k]$: $\frac{4\pi k^2 dk}{(2\pi/L)^3} = \frac{V}{(2\pi)^3} 4\pi k^2 dk$

↳ Same result

Scattering off a bound particle



→ Scattering center is a particle A bound by the potential W
Beam particles scatter off the potential V generated by the particle A and are not sensitive to potential W (which is related to a different type of interaction)

↳ example: <u>electron - proton scattering</u> ("deep inelastic scattering")
- protons are bound states made of quarks due to the strong nuclear force
- electrons do not feel the the strong force and only interact via the electromagnetic force due to the electric charge of the quarks.

→ We treat the potential V perturbatively.

For $V=0$: 2 decoupled systems →
- free particles (beam): $\left(-\frac{\vec{\nabla}^2}{2\mu} - \frac{k^2}{2\mu}\right)\phi_{\vec{k}}(\vec{x}_A) = 0$
- bound particle A (target): $\left(-\frac{\vec{\nabla}^2}{2M} + W(\vec{x}_B) - E_n\right)\psi_n(\vec{x}_B) = 0$

Hilbert space: direct product of the free and bound particle Hilbert spaces

→ We assume that the bound particle A is initially in its ground state $|\psi_0\rangle$, and we extend (<u>without proof</u>) the scattering formula for this case.

<u>Born level T matrix element</u>

incoming state: $|\vec{k}_i\rangle \otimes |\psi_0\rangle = |\vec{k}_i, \psi_0\rangle$

outgoing state: $\langle \vec{k}_f| \otimes \langle \psi_n| = \langle \vec{k}_f, \psi_n|$ ← $n = 0, 1, 2, \ldots$ (bound particle may be excited due to scattering)

$|\psi_n\rangle$ normalized: $\langle \psi_n|\psi_n\rangle = 1$

↳ $\langle \vec{k}_f, \psi_n| -V |\vec{k}_i, \psi_0\rangle$

$$= -\frac{1}{(2\pi)^3}\int d^3\vec{x}_A\, d^3\vec{x}_B\, e^{-i\vec{k}_f\vec{x}_A}\, \psi_n^*(\vec{x}_B)\, V(\vec{x}_A-\vec{x}_B)\, e^{i\vec{k}_i\vec{x}_A}\, \psi_0(\vec{x}_B)$$

$$= -\frac{1}{(2\pi)^3}\int d^3\vec{x}_A\, e^{-i\vec{k}_f\vec{x}_A}\underbrace{\left[\int d^3\vec{x}_B\, \psi_n^*(\vec{x}_B)\, V(\vec{x}_A-\vec{x}_B)\, \psi_0(\vec{x}_B)\right]}\, e^{i\vec{k}_i\vec{x}_A}$$

<u>$n=0$:</u> particle A not excited
→ $|\vec{k}_f| = |\vec{k}_i|$ elastic scattering

$$V_{eff}(\vec{x}_A) = \int d^3\vec{x}_B\, |\psi_0(\vec{x}_B)|^2\, V(\vec{x}_A-\vec{x}_B)$$

"averaged potential seen by beam particles"

↳ $$d\sigma = \frac{1}{|\vec{j}_{in}|}\,|\langle \vec{k}_f| -V_{eff}|\vec{k}_i\rangle|^2\,(2\pi)\,\delta(E_f-E_i)\,d^3\vec{k}_f$$

$$\frac{d\sigma}{d\Omega} = (2\pi)^4\mu^2\,|\tilde{V}_{eff}(\vec{k}_f-\vec{k}_i)|^2$$

$n \neq 0$: inelastic scattering with excitation of scattering center
$E_{k_f} + E_n = E_{k_i} + E_0$ (energy conservation)

$\hookrightarrow$ $\langle \vec{k}_f, \psi_n | -V | \vec{k}_i, \psi_0 \rangle$ $\quad \vec{x} = \vec{x}_A - \vec{x}_B \quad , \vec{q} = \vec{k}_f - \vec{k}_i$ ("momentum transfer")

$$= -\frac{1}{(2\pi)^3} \int d^3\vec{x}\, d^3\vec{x}_B\, e^{-i(\vec{k}_f - \vec{k}_i)(\vec{x} + \vec{x}_B)} \psi_n^*(\vec{x}_B) V(\vec{x}) \psi_0(\vec{x}_B)$$

$$= \underbrace{-\frac{1}{(2\pi)^3} \int d^3\vec{x}\, e^{-i\vec{q}\vec{x}} V(\vec{x})}_{\text{"free T matrix element"}} \times \underbrace{\int d^3\vec{x}_B\, e^{-i\vec{q}\vec{x}_B} \psi_n^*(\vec{x}_B) \psi_0(\vec{x}_B)}_{=: F_{n0}(\vec{k}_f - \vec{k}_i) = F_{n0}(\vec{q})}$$

"structure function" or "form factor"

contains information on the bound state properties of the target

$$\hookrightarrow \quad d\sigma = \frac{1}{|\vec{j}_{in}|} |\langle \vec{k}_f | -V | \vec{k}_i \rangle|^2 |F_{n0}(\vec{k}_f - \vec{k}_i)|^2 (2\pi) \delta(E_f + E_n - E_i - E_0)\, d^3\vec{k}_f$$

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \mu^2 |\tilde{V}(\vec{k}_f - \vec{k}_i)|^2 |F_{n0}(\vec{k}_f - \vec{k}_i)|^2 \qquad (k_f^2 = k_i^2 + 2\mu(E_0 - E_n))$$

$$= \left(\frac{d\sigma}{d\Omega}\right)\Big|_{free} |F_{n0}(\vec{k}_f - \vec{k}_i)|^2$$

$\longrightarrow$ One can learn a lot about the bound state structure if $(d\sigma/d\Omega)|_{free}$ is known.

Target disintegration: In case of inelastic scattering it may also be possible that the bound particle is broken out of the bound state and is a free particle after the scattering.

$\hookrightarrow$ 2 modifications: (a) $\psi_n^*(\vec{x}_B) \longrightarrow \phi^*_{\vec{k}_{fA}}(\vec{x}_B) = \frac{1}{(2\pi)^{3/2}} e^{-i\vec{k}_{fA}\vec{x}_B}$:

$$|F_{n0}(\vec{k}_f - \vec{k}_i)|^2 \longrightarrow \frac{1}{(2\pi)^3} \left| \int d^3\vec{x}_B\, e^{-i(\vec{k}_f + \vec{k}_{fA} - \vec{k}_i)} \psi_0(\vec{x}_B) \right|^2 = |\tilde{\psi}_0(\vec{k}_f + \vec{k}_{fA} - \vec{k}_i)|^2$$

(b) add final state integration $d^3\vec{k}_{fA}$

$$\hookrightarrow \quad d\sigma = \frac{1}{|\vec{j}_{in}|} |\langle \vec{k}_f | -V | \vec{k}_i \rangle|^2 |\tilde{\psi}_0(\vec{k}_f + \vec{k}_{fA} - \vec{k}_i)|^2 (2\pi) \delta(E_f + E_{fA} - E_i - E_0)\, d^3\vec{k}_f\, d^3\vec{k}_{fA}$$

Note: We can also use the form factor parametrization for the elastic case

$$\hookrightarrow \quad F_{00}(\vec{q}^2) = \int d^3\vec{x}\, e^{-i\vec{q}\vec{x}} |\psi_0(\vec{x})|^2$$

For small scattering angles we have $\vec{q} = \vec{k}_f - \vec{k}_i \longrightarrow 0$

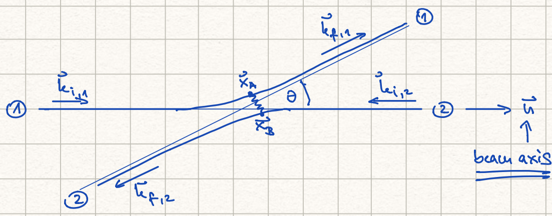
probability distribution $\rho(\vec{x})$ (normalized)

$$\hookrightarrow \quad F_{00}(\vec{q}^2) \approx \int d^3\vec{x} \left(1 - i\vec{q}\vec{x} - \frac{(\vec{q}\vec{x})^2}{2} + \ldots\right) |\psi_0(\vec{x})|^2$$

$$= 1 - i\vec{q} \underbrace{\int d^3\vec{x}\, \vec{x}\, \rho(\vec{x})}_{\substack{\text{dipole moment} \\ \text{(zero for sym. ground state)}}} - \frac{q^i q^j}{6} \underbrace{\int d^3\vec{x}\, \delta^{ij} |\vec{x}|^2 \rho(\vec{x})}_{\substack{\text{mean distance squared} \\ \text{of distribution } \rho(\vec{x})}} - \frac{q^i q^j}{2} \underbrace{\int d^3\vec{x} \left(x^i x^j - |\vec{x}|^2 \frac{\delta^{ij}}{3}\right) \rho(\vec{x})}_{\substack{\text{quadrupole moment} \\ \text{of distribution } \rho(\vec{x})}}$$

2 Particle Scattering

→ Head-on-head collision is the major collision type in modern collider experiments.



example: LHC : p-p collision
future Linear Collider : e^+e^- collisions
LEP : e^+e^- collisions
HERA : e^-p collisions

We consider elastic scattering $A(\vec{k}_i) + B(\vec{k}_i') \longrightarrow A(\vec{k}_f) + B(\vec{k}_f')$

We again proceed intuitively without proof.

Born level T matrix element

incoming state : $|\vec{k}_{i,1}\rangle \otimes |\vec{k}_{i,2}\rangle = |\vec{k}_{i,1}\,\vec{k}_{i,2}\rangle$
outgoing state : $\langle \vec{k}_{f,1}| \otimes \langle \vec{k}_{f,2}| = \langle \vec{k}_{f,1}\,\vec{k}_{f,2}|$

$\hookrightarrow \langle \vec{k}_{f,1}, \vec{k}_{f,2}| -V |\vec{k}_{i,1}, \vec{k}_{i,2}\rangle$

$$= -\frac{1}{(2\pi)^6}\int d^3\vec{x}_A\, d^3\vec{x}_B\, e^{-i\vec{k}_{f,1}\vec{x}_A} e^{-i\vec{k}_{f,2}\vec{x}_B} V(\vec{x}_A-\vec{x}_B)\, e^{i\vec{k}_{i,1}\vec{x}_A} e^{i\vec{k}_{i,2}\vec{x}_B} \qquad \vec{x} = \vec{x}_A - \vec{x}_B$$

$$= -\frac{1}{(2\pi)^3}\int d^3\vec{x}\, e^{-i(\vec{k}_{f,1}-\vec{k}_{i,1})\vec{x}}\, V(\vec{x}) \times \frac{1}{(2\pi)^3}\int d^3\vec{x}_B\, e^{-i(\vec{k}_{f,1}+\vec{k}_{f,2}-\vec{k}_{i,1}-\vec{k}_{i,2})\vec{x}_B}$$

$$= -\tilde{V}(\vec{k}_{f,1}-\vec{k}_{i,1})\,\delta^{(3)}(\vec{k}_{f,1}+\vec{k}_{f,2}-\vec{k}_{i,1}-\vec{k}_{i,2})$$

momentum conservation in addition to energy conservation

Problems: (a) How to deal with $|\langle \vec{k}_f, \vec{k}_f'| -V |\vec{k}_i, \vec{k}_i'\rangle|^2$?
(b) Both initial states are plane waves. ⟶ Norm of 'target' (A or B ?) $\neq 1$
What is the incoming probability current ?

We can resolve both problems by considering initial state wave packets:

$|\phi_{in}(\vec{k}_{in})\rangle = \int d^3\vec{q}\; \tilde{\phi}_{\vec{k}_{in}}(\vec{q})\,|\vec{q}\rangle$ $\qquad \tilde{\phi}_{\vec{k}}(\vec{q})$ mom space wave packet for a particle travelling in $\vec{k}$ direction exactly along the beam axis
→ strongly peaked at $\vec{q} \approx \vec{k}$

We impose $\langle \phi_{in}(\vec{k})|\phi_{in}(\vec{k})\rangle = 1$

$$\hookrightarrow \int d^3\vec{q}\, d^3\vec{q}'\, \tilde{\phi}^*_{\vec{k}}(\vec{q})\,\tilde{\phi}_{\vec{k}}(\vec{q}')\,\underbrace{\langle\vec{q}|\vec{q}'\rangle}_{\delta^{(3)}(\vec{q}-\vec{q}')} = \int d^3\vec{q}\,|\tilde{\phi}_{\vec{k}}(\vec{q})|^2 \stackrel{!}{=} 1$$

$\Rightarrow |\langle \vec{k}_{f_1}, \vec{k}_{f_2}| -V |\phi^1_{in}(\vec{k}_{i_1}), \phi^2_{in}(\vec{k}_{i_2})\rangle|^2\, d^3k_{f_1}\, d^3k_{f_2}$ = probability that the final state particles are scattered into momentum volume elements $d^3k_{f_1}\, d^3k_{f_2}$ when two normalized wave packets collide.

$\rightarrow$ Because we are now back to the scattering of <u>individual particles</u> we cannot easily use the probability current to properly normalize the cross section.

We have to get back to the basic definition of the cross section:

$$\frac{\sigma}{A} = \frac{N_{scatter}}{N_1 N_2}$$

$N_{scatter}$: # of events when scattering happened (within time T)

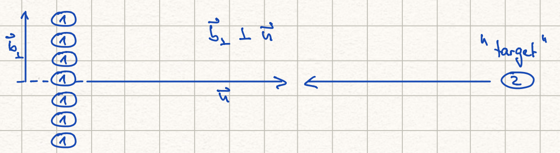
$N_{1/2}$: # of particles of type 1/2 in beams that are involved in scattering (within time T)

A : overlap area of the beams ($\perp$ to beam direction)

$A \gg$ size of wave packets

We now simplify the the situation of 1 target particle ② and a beam of particles ① : $\longrightarrow N_2 = 1$

We now must account for the fact that the wave packets can have any impact parameter $\vec b$ w.r.t. to the beam axis. We cannot distinguish the different situations and must sum over them.



shift operator for particle 1 wave packet

$$\rightarrow \; |\phi^1_{in}(\vec k_{i_1}), \phi^2_{in}(\vec k_{i_2})\rangle_{\vec b_\perp} = \int d^3k_1\, d^3k_2\; \tilde\phi_{\vec k_{i,1}}(\vec k_1)\, \tilde\phi_{\vec k_{i,2}}(\vec k_2)\; e^{-i\vec b_\perp \vec k_1}\, |\vec k_1, \vec k_2\rangle$$

$\vec b_\perp$: x and y components

$\vec n$: z-direction

The cross section is now determined from:

$$\sigma = \frac{N_{scatter}}{n_1}$$

$N_{scatter}$: # of events when scattering happened (within time T)

n_1 : area density ($\perp$ to beam direction) of type 1 particles in the beam (within time T)

$\rightarrow$ assumed constant

$$\Rightarrow \quad N_{scatter} \simeq \int d^2 b_\perp\; n_1 \times |\langle \vec k_{f_1}, \vec k_{f_2}| -V |\phi^1_{in}(\vec k_{i_1}), \phi^2_{in}(\vec k_{i_2})\rangle_{\vec b_\perp}|^2\, d^3k_{f_1}\, d^3k_{f_2}$$

kinematic constraints still have to be included

drops out in σ

We try the following ansatz

$$d\sigma = \int d^2 b_\perp \int d^3k_1\, d^3k_2\, d^3k_1'\, d^3k_2'\; \tilde\phi_{\vec k_{i,1}}(\vec k_1)\, \tilde\phi^*_{\vec k_{i,1}}(\vec k_1')\, \tilde\phi_{\vec k_{i,2}}(\vec k_2)\, \tilde\phi^*_{\vec k_{i,2}}(\vec k_2')\; e^{i\vec b_\perp(\vec k_1 - \vec k_1')}$$

$$\times \langle \vec k_{f,1}, \vec k_{f,2}| -V |\vec k_1, \vec k_2\rangle \left(\langle \vec k_{f,1}, \vec k_{f,2}| -V |\vec k_1', \vec k_2'\rangle\right)^*$$

$$\times (2\pi)\,\delta(E_{k_1} + E_{k_2} - E_{k_{f,1}} - E_{k_{f,2}})\; (2\pi)\,\delta(E_{k_1'} + E_{k_2'} - E_{k_{f,1}} - E_{k_{f,2}})\; d^3k_{f,1}\, d^3k_{f,2}$$

We use two E-conserving δ-fcts, because the matrix elements have different momenta. This appears ad hoc, but otherwise we cannot implement energy conservation for the wave packets. It is also meaningful for dimensional reasons ($\rightarrow \sigma \sim x^2 \sim k^{-2}$)

$\rightarrow$ Will be justified rigorously when we do <u>time-dependent perturbation theory</u>

$$= \int d^3k_1\, d^3k_2\, d^3k_1'\, d^3k_2'\; \tilde\varphi_{k_{i,1}}(k_1)\, \tilde\varphi^*_{k_{i,1}}(k_1')\, \tilde\varphi_{k_{i,2}}(k_2)\, \tilde\varphi^*_{k_{i,2}}(k_2') \; * (2\pi)^2 \underbrace{\delta(k_{1,x}-k_{1,x}')\,\delta(k_{1,y}-k_{1,y}')}_{a}$$

$$* \; \tilde V(k_{f,1}-k_1)\, \tilde V(k_{f,1}-k_1')\, \underbrace{\delta^{(3)}(k_{f,1}+k_{f,2}-k_1-k_2)}_{b}\, \underbrace{\delta^{(3)}(k_{f,1}+k_{f,2}-k_1'-k_2')}_{c}$$

$$* \; (2\pi)\,\delta(E_{k_1}+E_{k_2}-E_{k_{f,1}}-E_{k_{f,2}})\,(2\pi)\,\delta(E_{k_1'}+E_{k_2'}-E_{k_{f,1}}-E_{k_{f,2}})\; d^3k_{f,1}\, d^3k_{f,2}$$

We get: $(k_{1,x}', k_{1,y}')$ set to $(k_{1,x}, k_{1,y})$ due to (a)
$(k_{2,x}', k_{2,y}')$ set to $(k_{2,x}, k_{2,y})$ due to (b) with (c)

$\Rightarrow$ remaining prime integrals:

$$\int dk_{1,z}'\, dk_{2,z}'\; \delta(k_{1,z}'+k_{2,z}'-k_{f,1,z}-k_{f,2,z})\,\delta(E_{k_1'}+E_{k_2'}-E_{k_{f,1}}-E_{k_{f,2}})$$

$$= \int dk_{1,z}' \;\; \delta\Big(\frac{k_{1,x}'^2+k_{1,y}'^2+k_{1,z}'^2}{2\mu_1} + \frac{k_{2,x}'^2+k_{2,y}'^2+(k_{1,z}'-k_{f,1,z}-k_{f,2,z})^2}{2\mu_2} - E_{k_{f,1}} - E_{k_{f,2}}\Big)$$

zero for $k_{1,z}' = k_{1,z}$ $\Rightarrow$ $\delta(\dots) = \delta\Big(\underbrace{\frac{d}{dk_{1,z}'}[\dots]}\,(k_{1,z}'-k_{1,z})\Big)$

$$= \frac{k_{1,z}}{\mu_1} + \frac{1}{\mu_2}(k_{1,z}-k_{f,1,z}-k_{f,2,z}) = \frac{k_{1,z}}{\mu_1} - \frac{k_{2,z}}{\mu_2}$$

$$= \frac{1}{\left|\frac{k_{1,z}}{\mu_1} - \frac{k_{2,z}}{\mu_2}\right|}$$ (setting $k_{1,z}'$ to $k_{1,z}$ and $k_{2,z}'$ to $k_{2,z}$)

This is just the relative flux of the 2 incoming beams!

$$= \int d^3k_1\, d^3k_2\; |\tilde\varphi_{k_{i,1}}(k_1)|^2\, |\tilde\varphi_{k_{i,2}}(k_2)|^2\, \frac{(2\pi)^3}{\left|\frac{k_{1,z}}{\mu_1}-\frac{k_{2,z}}{\mu_2}\right|}$$

$$* \; |\tilde V(k_{f,1}-k_1)|^2\, \delta^{(3)}(k_{f,1}+k_{f,2}-k_1-k_2)\,(2\pi)\,\delta(E_{k_1}+E_{k_2}-E_{k_{f,1}}-E_{k_{f,2}})\; d^3k_{f,1}\, d^3k_{f,2}$$

We now use that the wave packets $|\tilde\varphi_{k_{i,1}}(k_1)|^2$ and $|\tilde\varphi_{k_{i,2}}(k_2)|^2$ are strongly peaked at $k_{i,1}$ and $k_{i,2}$, respectively, and that the rest of the dependence on k_1 and k_2 is smooth

$$\approx \overbrace{\int d^3k_1\, d^3k_2\; |\tilde\varphi_{k_{i,1}}(k_1)|^2\, |\tilde\varphi_{k_{i,2}}(k_2)|^2}^{=1}\; \frac{(2\pi)^3}{\left|\frac{k_{i,1,z}}{\mu_1}-\frac{k_{i,2,z}}{\mu_2}\right|}$$

$$* \; |\tilde V(k_{f,1}-k_{i,1})|^2\, \delta^{(3)}(k_{f,1}+k_{f,2}-k_{i,1}-k_{i,2})\,(2\pi)\,\delta(E_{k_{i,1}}+E_{k_{i,2}}-E_{k_{f,1}}-E_{k_{f,2}})\; d^3k_{f,1}\, d^3k_{f,2}$$

Final result for 2-particle scattering cross section (in any frame)

$$\boxed{d\sigma = \frac{1}{|j_{in,1}-j_{in,2}|}\, |\tilde V(k_{f,1}-k_{i,1})|^2\, \delta^{(3)}(k_{f,1}+k_{f,2}-k_{i,1}-k_{i,2}) \; * \; (2\pi)\,\delta(E_{k_{i,1}}+E_{k_{i,2}}-E_{k_{f,1}}-E_{k_{f,2}})\; d^3k_{f,1}\, d^3k_{f,2}} \qquad j_{in,1/2} = \frac{k_{i,1/2}}{(2\pi)^3\mu_{1/2}} \qquad (*)$$

Comments:

Stationary target limit:

For $\mu_2 \to \infty$ we have $\vec{v}_{i,2}, \vec{v}_{f,2} \to 0$, $E_{ki,2}, E_{kf,2} \to 0$, $\vec{j}_{in,2} \to 0$.
Particle 2 does not move at all.

$$\leadsto d\sigma = \frac{1}{|\vec{j}_{in,1}|} |\tilde{v}(\vec{k}_{f,1} - \vec{k}_{i,1})|^2 \, \delta^{(3)}(\vec{k}_{f,1} + \vec{k}_{f,2} - \vec{k}_{i,1} - \vec{k}_{i,2}) \, (2\pi) \, \delta(\underbrace{E_{k_{i,1}} - E_{kf,1}}_{|\vec{k}_{i,1}| = |\vec{k}_{f,1}| \text{ elastic scattering!}}) \, d^3\vec{k}_{f,1} \, d^3\vec{k}_{f,2}$$

Particle 2 final state momentum can have any size $\vec{k}_{f,2}$ and does not affect the cross section.
We can integrate over it.

$$\leadsto d\sigma = \frac{1}{|\vec{j}_{in,1}|} |\tilde{v}(\vec{k}_{f,1} - \vec{k}_{i,1})|^2 \, (2\pi) \, \delta(E_{k_{i,1}} - E_{kf,1}) \, d^3\vec{k}_{f,1}$$

We recover exactly the cross section of elastic scattering of particle 1
off the stationary potential caused by particle 2 (which is infinitely heavy).

$\leadsto$ Our ad hoc manipulations are fully consistent (and in fact completely correct).

Differential cross sections

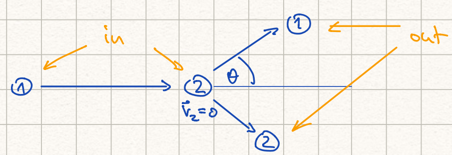
From Eq (*) we have plenty of options to define differential cross sections.
We can pick any variable that we want as long as it can be computed from the final state momenta $\vec{k}_{f,1}$ and $\vec{k}_{f,2}$:

$$\frac{d\sigma}{dX} = \int d^3\vec{k}_{f,1} \, d^3k_{f,2} \, \frac{1}{|\vec{j}_{in,1} - \vec{j}_{in,2}|} |\tilde{v}(\vec{k}_{f,1} - \vec{k}_{i,1})|^2 \, \delta^{(3)}(\vec{k}_{f,1} + \vec{k}_{f,2} - \vec{k}_{i,1} - \vec{k}_{i,2})$$
$$* \, (2\pi) \, \delta(E_{k_{i,1}} + E_{k_{i,2}} - E_{kf,1} - E_{kf,2}) \, \delta(X - x(\vec{k}_{f,1}, \vec{k}_{f,2}))$$

Also multi-differential cross sections are possible

$$\frac{d\sigma}{dX_1 \, dX_2 \cdots} = \int d^3\vec{k}_{f,1} \, d^3k_{f,2} \, \frac{1}{|\vec{j}_{in,1} - \vec{j}_{in,2}|} |\tilde{v}(\vec{k}_{f,1} - \vec{k}_{i,1})|^2 \, \delta^{(3)}(\vec{k}_{f,1} + \vec{k}_{f,2} - \vec{k}_{i,1} - \vec{k}_{i,2})$$
$$* \, (2\pi) \, \delta(E_{k_{i,1}} + E_{k_{i,2}} - E_{kf,1} - E_{kf,2}) \, \delta(X_1 - x_1(\vec{k}_{f,1}, \vec{k}_{f,2})) \, \delta(X_2 - x_2(\vec{k}_{f,1}, \vec{k}_{f,2})) \cdots$$

Fixed target frame:



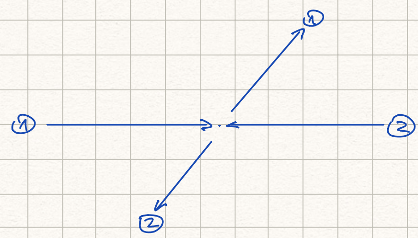
One particle (let's say 2) has $\vec{k}_{i,2} = 0$ before scattering: $\vec{j}_{in,2} = 0$

Due to energy and momentum conservation $\vec{k}_{f,1}, \vec{k}_{f,2} \neq 0$ if $\theta \neq 0$

Center of mass frame:

Initial state momenta vanish : $\vec{k}_{i,1} + \vec{k}_{i,2} = 0$

$$\rightsquigarrow \quad \vec{k}_{f,1} + \vec{k}_{f,2} = 0$$



Used e.g. at the LHC.

Cross section in different reference frames:

→ Total cross section σ_{tot} is frame - independent. (Areas are frame-independent.)

$$\sigma_{tot} = \frac{(I_{in} - I_{out}) \cdot (\text{beam area})}{I_{in}}$$

Intensities can change, but only globally by an overall factor.

That σ_{tot} is frame-independent is also true in the relativistic case (although areas are not frame-independent.)

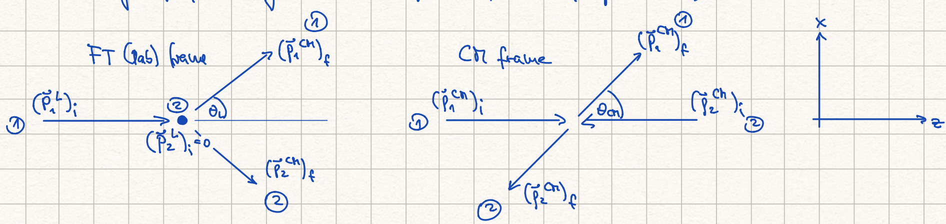
→ Differential cross sections are in general frame-dependent when they depend on kinematic quantities that are frame-dependent.

Example: Angular differential cross section

$$\left.\begin{array}{ll} \text{Solid angles frame 1:} & \phi_1, \theta_1 \\ \text{Solid angles frame 2:} & \phi_2, \theta_2 \end{array}\right\} \quad \begin{array}{l} \phi_1 = \phi_1(\phi_2, \theta_2) \\ \theta_1 = \theta_1(\phi_2, \theta_2) \end{array}$$

$$\rightsquigarrow \quad \left.\frac{d\sigma}{d\phi_1\, d\cos\theta_1}\right|_{\text{frame 1}} = \left|\frac{d(\phi_2, \cos\theta_2)}{d(\phi_1, \cos\theta_1)}\right| \times \left.\frac{d\sigma}{d\phi_2\, d\cos\theta_2}\right|_{\text{frame 2}}$$

Consider change of fixed target to center of mass frame (for particle 1)



FT frame moves with velocity $(\vec{v}_2^{\,CM})_i$ w.r.t. the CM frame

$\Longrightarrow$ velocities in the FT frame : $\vec{v}^{L} = \vec{v}^{CM} - (\vec{v}_2^{CM})_i$

momentum conservation : $\mu_1 (\vec{v}_1^{CM})_i = -\mu_2 (\vec{v}_2^{CM})_i \iff (\vec{v}_2^{CM})_i = -\frac{\mu_1}{\mu_2} (\vec{v}_1^{CM})_i$

$\hookrightarrow \phi_L = \phi_{CM}$

$$\tan\theta_L = \frac{(v_{1,x}^{L})_f}{(v_{1,z}^{L})_f} = \frac{(v_{1,x}^{CM})_f}{(v_{1,z}^{CM})_f + \frac{\mu_1}{\mu_2} (v_{1,z}^{CM})_i} \qquad (v_{1,z}^{CM})_i = |(\vec{v}_1^{CM})_i| = |(v_1^{CM})_f|$$

$$= \frac{(v_{1,x}^{CM})_f}{(v_{1,z}^{CM})_f + \frac{\mu_1}{\mu_2} |(\vec{v}_1^{CM})_f|} = \frac{\sin\theta_{CM}}{\cos\theta_{CM} + \frac{\mu_1}{\mu_2}}$$

$$\iff \cos\theta_L = \frac{\mu_1 + \mu_2 \cos\theta_{CM}}{\sqrt{\mu_1^2 + \mu_2^2 + 2\mu_1\mu_2 \cos\theta_{CM}}}$$

<u>Special case :</u> $\mu_1 = \mu_2 = \mu \quad \Longrightarrow \quad \tan\theta_L = \frac{\sin\theta_{CM}}{\cos\theta_{CM} + 1} = \tan\frac{\theta_{CM}}{2}$

$\hookrightarrow \theta_L = \frac{\theta_{CM}}{2} \quad , \quad \phi_L = \phi_{CM}$

$$\frac{d(\phi_{CM}, \cos\theta_{CM})}{d(\phi_L, \cos\theta_L)} = \frac{d\cos\theta_{CM}}{d\cos\theta_L} = \frac{d\cos(2\theta_L)}{d\cos(\theta_L)} = \frac{-\sin(2\theta_L)\, 2\, d\theta_L}{-\sin(\theta_L)\, d\theta_L} = \frac{2\sin(2\theta_L)}{\sin(\theta_L)}$$

$$= \frac{4\sin\theta_L \cos\theta_L}{\sin\theta_L} = 4\cos\theta_L$$

$$\Longrightarrow \frac{d\sigma}{d\Omega_L} = \left(4\cos\left(\frac{\theta_{CM}}{2}\right)\right) \frac{d\sigma}{d\Omega_{CM}}$$

2.8. Time-Dependent Perturbation Theory

Propagator / Green's function method

↳ time-dependent Schrödinger equation (spin-less particle in time-dependent potential):

$$\left(i\frac{\partial}{\partial t} - H\right)\psi(\vec{x},t) = 0 \quad , \quad H = \frac{\vec{p}^{\,2}}{2\mu} + V(\vec{x},t) = H_0 + V(\vec{x},t) \qquad \longrightarrow \text{Exercises}$$

↳ Retarded Green's function for the free Schrödinger equation (propagator):

Configuration space: $\left(i\frac{\partial}{\partial t} - H_0\right) G_0(x,x') = i\,\delta(t-t')\,\delta^{(3)}(\vec{x}-\vec{x}\,')$

$$G_0(x,x') = \int \frac{d^4q}{(2\pi)^4}\frac{d^4q'}{(2\pi)^4}\, e^{-iq.x}\, \frac{i(2\pi)^4\delta^{(4)}(q-q')}{q_0 - \frac{\vec{q}^{\,2}}{2\mu}+i\epsilon}\, e^{+iq'.x'} \qquad \langle\vec{x}|\vec{q}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\vec{q}\vec{x}}$$

$$= \Theta(t-t')\int d^3\vec{q}\,\langle\vec{x}|\vec{q}\rangle\, e^{-i\frac{\vec{q}^{\,2}}{2\mu}(t-t')}\langle\vec{q}|\vec{x}\,'\rangle \qquad q.x := q_0 t - \vec{q}\vec{x}$$

$$= \frac{\Theta(t-t')}{[2\pi i(t-t')/\mu]^{3/2}}\exp\left(\frac{i\mu(\vec{x}-\vec{x}\,')^2}{2(t-t')}\right) \qquad q^\mu = (q_0,\vec{q}) = (q_0,q_1,q_2,q_3)$$

Momentum space: $\left(q_0 - \frac{\vec{q}^{\,2}}{2\mu}\right)\tilde{G}_0(q,q') = i(2\pi)^4\delta^{(4)}(q-q')$

$$\tilde{G}_0(q,q') = \frac{i(2\pi)^4\delta^{(4)}(q-q')}{q_0 - \frac{\vec{q}^{\,2}}{2\mu}+i\epsilon}$$

Comments:

- We use the 4-vector notation: ⟶ Essential when we consider relativistic physics.

$x^\mu = (t,\vec{x})$, $q^\mu = (q_0,\vec{q})$ (contravariant 4-vector)

$x_\mu = (t,-\vec{x})$, $q_\mu = (q_0,-\vec{q})$ (covariant 4-vector)

energy ⤴ ⤴ momentum

$$x.q =: x^\mu q_\mu = x_\mu q^\mu = q_0 t - \vec{q}\vec{x}$$

Abbreviated notation: $f(x) = f(t,\vec{x})$, $\tilde{f}(q) = \tilde{f}(q_0,\vec{q})$, $\delta^{(4)}(x-x') = \delta(t-t')\delta^{(3)}(\vec{x}-\vec{x}\,')$

- $G_0(x,x') = G_0(t,\vec{x}|t',\vec{x}\,')$ is a "forward time" evolution operator: ⤳ causality implemented!

$$G_0(t,\vec{x}|t',\vec{x}\,') = \langle\vec{x}|\,\Theta(t-t')e^{-iH_0(t-t_0)}|\vec{x}\,'\rangle \neq U(t,t_0) = \exp(-iH_0(t-t_0))$$

- Given $\psi(t_0,\vec{x})$ we can use $G_0(x,x')$ to determine $\psi(t>t_0,\vec{x}) = \int d^3\vec{x}\,'\, G_0(t,\vec{x}|t_0,\vec{x}\,')\psi(t_0,\vec{x}\,')$

Check: $(i\partial_t - H_0)\psi(t,\vec{x}) = \int d^3\vec{x}\,'\,[i\partial_t - H_0]G_0(t,\vec{x}|t_0,\vec{x}\,')\psi(t_0,\vec{x}\,') = \int d^3\vec{x}\,'\,[i\delta(t-t_0)\delta^{(3)}(\vec{x}-\vec{x}\,')]\psi(t_0,\vec{x}\,')$

$$= i\delta(t-t_0)\psi(t_0,\vec{x}) = 0 \quad (\text{for } t>t_0)$$

- $G_0(x,x')$ "propagates" a particle located at $x'^\mu = (t', \vec{x}')$ dynamically (i.e. due to H_0) to the location $x^\mu = (t > t', \vec{x})$
  ↳ origin of name propagator

- $\tilde{G}_0(q,q') \sim \delta^{(4)}(q-q') = \delta(q_0 - q_0')\,\delta^{(3)}(\vec{q}-\vec{q}')$
  ↳ Implementation of energy-momentum conservation.

- $G_0(t_f, \vec{x}_f \,|\, t_i, \vec{x}_i) = \int d^3\vec{x}\; G_0(t_f, \vec{x}_f \,|\, t, \vec{x})\, G_0(t, \vec{x} \,|\, t_i, \vec{x}_i)$
  for $t_i < t < t_f$

Time-dependent scattering problem

→ Physical setup for time-dependent scattering ("Asymptotic states") → We consider again elastic 1 particle scattering for simplicity.

$t_i \to -\infty$: Wave starts as incoming free wave with fixed momentum $\vec{k}_i$. (It does not feel yet the potential which has finite range.)

$t_f \to +\infty$: Wave is detected as outgoing free wave with fixed momentum $\vec{k}_f$. (It does not feel any more the potential which has finite range.)

$\infty \;\hat{=}\;$ "Much larger as the time span in which the interaction takes place." (Frequently one can really calculate with times at $\pm\infty$, but one has to be aware of the approximation)

↳ When problems arise use (a) localized wave packets ⊕ finite range potential
(b) $t_{i/f} = \mp T$, then limit $T \to \infty$

→ "S-matrix element" $\hat{=}$ Amplitude that a free incoming particle at $t_i \to -\infty$ with momentum $\vec{k}_i$ is later at $t_f \to +\infty$ detected as a free outgoing particle with momentum $\vec{k}_f$.

↳ $\varphi_{in}(t_i, \vec{x}) = \frac{1}{(2\pi)^{3/2}}\, e^{-iE_i t_i}\, e^{i\vec{k}_i \vec{x}} \qquad E_i = \frac{k_i^2}{2\mu} \qquad$ (initial condition)

$\varphi_{out}(t_f, \vec{x}) = \frac{1}{(2\pi)^{3/2}}\, e^{-iE_f t_f}\, e^{i\vec{k}_f \vec{x}} \qquad E_f = \frac{k_f^2}{2\mu} \qquad$ (measurement final state)

↳ We want the time-evolved state at $t = t_f$ that starts as $\varphi_{in}(t_i, \vec{x})$: $\varphi_{in}^{(+)}(t_f, \vec{x})$

$$\left(i\frac{\partial}{\partial t} - H_0 - V(t,\vec{x})\right)\varphi_{in}^{(+)}(t,\vec{x}) = 0 \quad \text{with} \quad \varphi_{in}^{(+)}(t_i,\vec{x}) = \varphi_{in}(t_i,\vec{x})$$

$$\Longleftrightarrow \left(i\frac{\partial}{\partial t} - H_0\right)\varphi_{in}^{(+)}(t,\vec{x}) = V(t,\vec{x})\,\varphi_{in}^{(+)}(t,\vec{x})$$

$$\Rightarrow \quad \psi_{in}^{(+)}(t_f,\vec{x}) = \int d^3\vec{x}'\, G_0(t_f,\vec{x}\,|\,t_i,\vec{x}')\, \psi_{in}(t_i,\vec{x}') \quad \leftarrow \text{homogeneous solution}$$

$$- i \int_{t_i}^{t_f} dt' \int d^3\vec{x}'\, G_0(t_f,\vec{x}\,|\,t',\vec{x}')\, V(t',\vec{x}')\, \psi_{in}^{(+)}(t',\vec{x}') \quad \leftarrow \text{implicit}$$

$$= \int d^3\vec{x}'\, G_0(t_f,\vec{x}\,|\,t_i,\vec{x}')\, \psi_{in}(t_i,\vec{x}')$$

$$- i \int_{t_i}^{t_f} dt' \int d^3\vec{x}'\, d^3\vec{x}''\, G_0(t_f,\vec{x}\,|\,t',\vec{x}')\, V(t',\vec{x}')\, G_0(t',\vec{x}'\,|\,t_i,\vec{x}'')\, \psi_{in}(t_i,\vec{x}'') \quad \leftarrow \text{Born approx.}$$

$$+ (-i)^2 \int_{t_i}^{t_f} dt' \int_{t_i}^{t'} dt'' \int d^3\vec{x}'\, d^3\vec{x}''\, d^3\vec{x}'''\, G_0(t_f,\vec{x}\,|\,t',\vec{x}')\, V(t',\vec{x}')\, G_0(t',\vec{x}'\,|\,t'',\vec{x}'')$$

$\uparrow$ (t_i also possible)

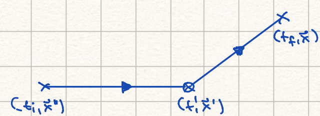
$$\times\ V(t'',\vec{x}'')\, G_0(t'',\vec{x}''\,|\,t_i,\vec{x}''')\, \psi_{in}(t_i,\vec{x}''')$$

$$+ \ldots$$

S-matrix element:

$$S_{\vec{k}_f,\vec{k}_i} = \int d^3\vec{x}\; \psi^*_{out}(t_f,\vec{x})\, \psi^{(+)}_{in}(t_f,\vec{x})$$

$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i) \; - 2\pi i\, \underbrace{\delta(E_f - E_i)}\; T_{\vec{k}_f,\vec{k}_i} \quad \leftarrow \text{T matrix element}$$



$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i)$$

Configuration space

$$+ (-i) \int_{t_i}^{t_f} dt'\; d^3\vec{x}\, d^3\vec{x}'\, d^3\vec{x}''\; \psi^*_{out}(t_f,\vec{x})\, G_0(t_f,\vec{x}\,|\,t',\vec{x}')\, V(t',\vec{x}')\, G_0(t',\vec{x}'\,|\,t_i,\vec{x}'')\, \psi_{in}(t_i,\vec{x}'')$$

$$+ \ldots$$

$$\left[\ \int d^3\vec{x}\; \psi^*_{out}(t_f,\vec{x})\, G_0(t_f,\vec{x}\,|\,t',\vec{x}') = \theta(t_f - t') \int d^3\vec{q}\, d^3\vec{x}\; \langle \vec{k}_f|\vec{x}\rangle\langle\vec{x}|\vec{q}\rangle\, e^{-i\left(\frac{\vec{q}^2}{2\mu} - \frac{\vec{k}_f^2}{2\mu}\right)t}\, e^{i\frac{\vec{q}^2}{2\mu}t'} \langle \vec{q}|\vec{x}'\rangle \right.$$

$$\left. = \theta(t_f - t')\, e^{i\frac{\vec{k}_f^2}{2\mu}t'} \langle \vec{k}_f|\vec{x}'\rangle = \theta(t_f - t')\, \psi^*_{out}(t',\vec{x}') \right.$$

$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i)$$

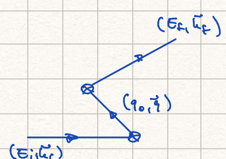
$$+ (-i) \int_{t_i}^{t_f} dt'\, d^3\vec{x}'\; \psi^*_{out}(t',\vec{x}')\, V(t',\vec{x}')\, \psi_{in}(t',\vec{x}')$$

$$+ (-i)^2 \int_{t''}^{t_f} dt' \int_{t_i}^{t_f} dt'' \int d^3\vec{x}' \int d^3\vec{x}''\; \psi^*_{out}(t',\vec{x}')\, V(t',\vec{x}')\, G_0(t',\vec{x}'\,|\,t'',\vec{x}'')\, V(t'',\vec{x}'')\, \psi_{in}(t'',\vec{x}'')$$

$$+ \ldots$$

Only these terms contribute to scattering

$$= \delta^{(3)}(\vec{k}_f - \vec{k}_i)$$

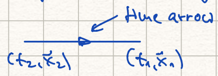


$$+ (-i)\, \tilde{V}(E_f - E_i,\, \vec{k}_f - \vec{k}_i)$$

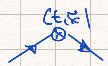
$$+ (-i)^2 \int \frac{d^4q}{(2\pi)}\, \tilde{V}(E_f - q_0,\, \vec{k}_f - \vec{q})\, \frac{i}{q_0 - \frac{\vec{q}^2}{2\mu} + i\epsilon}\, \tilde{V}(q_0 - E_i,\, \vec{q} - \vec{k}_i)$$

$$+ \ldots$$

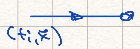
Configuration space Feynman rules:



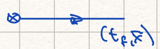
$G_0(t_1,\vec{x}_1 | t_2,\vec{x}_2)$ propagator



$-i\, V(t,\vec{x})$ vertex factor



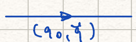
$\Psi_{in}(t_i,\vec{x})$ incoming wave



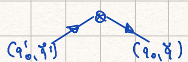
$\Psi^*_{out}(t_f,\vec{x})$ outgoing wave

Additional rules : * write down terms in reverse time-direction
* integrate over all intermediate t and $\vec{x}$

Momentum space Feynman rules:



$$\frac{i}{q_0 - \frac{\vec{q}^2}{2\mu} + i\epsilon}$$ propagator



$$(-i)\, \underbrace{\tilde{V}(q_0 - q_0', \vec{q} - \vec{q}\,')}$$ vertex factor

$$= \frac{1}{(2\pi)^2} \int dt\, d^3\vec{x}\; e^{-i q.x}\, V(t,\vec{x}) \qquad q.x = q_0 t - \vec{q}\vec{x}$$

Additional rules : * write down terms in reverse time-direction
* integrate over all intermediate momenta : $\int \frac{d^4 q}{(2\pi)}$

Trivial application: time-independent potential for 2-2 scattering

$$V(t,\vec{x}) = V(\vec{x})$$

$$\hookrightarrow \tilde{V}(q_0,\vec{q}) = \frac{1}{(2\pi)^3} \int dt\, e^{-i q_0 t} \int d^3\vec{x}\, e^{i\vec{q}\vec{x}}\, V(\vec{x}) = (2\pi)\,\delta(q_0)\, \tilde{V}(\vec{q})$$

↑ energy conservation!

$\hookrightarrow$ This justifies precisely our treatmen for 2-particle scattering in Sec 2.7.

Everything is derived in analogy to 1-particle scattering

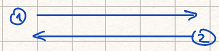
$$\Psi_{in}(t_i,\vec{x}_1,\vec{x}_2) = \frac{1}{(2\pi)^3}\, e^{-i(E_{i1}+E_{i2})t_i}\, e^{i\vec{k}_{i1}\vec{x}_1}\, e^{i\vec{k}_{i2}\vec{x}_2} \qquad E_{i1,2} = \frac{k_{i1,2}^2}{2\mu_{1,2}} \qquad \text{(initial condition)}$$

$$\Psi_{out}(t_f,\vec{x}_1,\vec{x}_2) = \frac{1}{(2\pi)^3}\, e^{-i(E_{f1}+E_{f2})t_f}\, e^{i\vec{k}_{f1}\vec{x}_1}\, e^{i\vec{k}_{f2}\vec{x}_2} \qquad E_{f1,2} = \frac{k_f^2}{2\mu_{1,2}} \qquad \text{(measurement final state)}$$

S-matrix element for $2 \rightarrow 2$ scattering: $\vec{k}_{i_1}, \vec{k}_{i_2} \longrightarrow \vec{k}_{f_1}, \vec{k}_{f_2}$ (only Born approximation)

$$S_{\vec{k}_{i_1},\vec{k}_{i_2} \to \vec{k}_{f_1},\vec{k}_{f_2}} = \int d^3\vec{x}_1\, d^3\vec{x}_2\; \psi^*_{out}(t_f,\vec{x}_1,\vec{x}_2)\, \psi^{(+)}_{in}(t_f,\vec{x}_1,\vec{x}_2)$$

$$= \delta^{(3)}(\vec{k}_{f_1}-\vec{k}_{i_1})\,\delta^{(3)}(\vec{k}_{f_2}-\vec{k}_{i_2}) \quad \longleftarrow \text{ no scattering}$$



$$+ (-i) \underbrace{\int_{t_i}^{t_f} dt\, d^3\vec{x}_1\, d^3\vec{x}_2\; \psi^*_{out}(t,\vec{x}_1,\vec{x}_2)\, V(\vec{x}_1-\vec{x}_2)\, \psi_{in}(t,\vec{x}_1,\vec{x}_2)} \qquad \vec{x} = \vec{x}_1 - \vec{x}_2$$

$$= \frac{1}{(2\pi)^6}\int dt\, d^3\vec{x}\, d^3\vec{x}_2\; e^{i(E_{f_1}+E_{f_2}-E_{i_1}-E_{i_2})t}\, e^{-i(\vec{k}_{f_1}-\vec{k}_{i_1})\vec{x}}\, V(\vec{x})\, e^{-i(\vec{k}_{f_1}+\vec{k}_{f_2}-\vec{k}_{i_1}-\vec{k}_{i_2})\vec{x}_2}$$

$$= 2\pi\, \delta(E_{f_1}+E_{f_2}-E_{i_1}-E_{i_1})\, \delta^{(3)}(\vec{k}_{f_1}+\vec{k}_{f_2}-\vec{k}_{i_1}-\vec{k}_{i_2})\, \tilde{V}(\vec{k}_{f_1}-\vec{k}_{i_1})$$

Generic cross section formula:

$$d\sigma = \int d^2\vec{b}_\perp \int d^3\vec{k}_1\, d^3\vec{k}_2\, d^3\vec{k}_1'\, d^3\vec{k}_2'\; \tilde{\varphi}_{\vec{k}_{i,1}}(\vec{k}_1)\, \tilde{\varphi}^*_{\vec{k}_{i,1}}(\vec{k}_1')\, \tilde{\varphi}_{\vec{k}_{i,2}}(\vec{k}_2)\, \tilde{\varphi}^*_{\vec{k}_{i,2}}(\vec{k}_2')\, e^{i\vec{b}_\perp(\vec{k}_1-\vec{k}_1')}$$

$$\times \left(S_{\vec{k}_1,\vec{k}_2 \to \vec{k}_{f_1},\vec{k}_{f_2}}\right)\left(S_{\vec{k}_1',\vec{k}_2' \to \vec{k}_{f_1},\vec{k}_{f_2}}\right)^* d^3\vec{k}_{f,1}\, d^3\vec{k}_{f,2}$$

$\rightarrow$ Leads exactly to the final formula for the $2 \rightarrow 2$ cross section we have already derived in Sec 2.7. $\longrightarrow$ page 04/06/2018 (13)

2.9. The Interaction Picture

→ So far we have used the Schrödinger picture to solve the scattering problem.

→ The interaction picture is a more efficient way to formulate perturbation theory for time-dependent problems. Basis of canonical formulation of quantum field theory.
$\rightarrow$ But final results of course equivalent to what we have obtained previously

Recall: Time-evolution operator $U(t_2,t_1) = e^{-iH(t_2-t_1)}$ for time-independent H

$\rightarrow$ $t_2 > t_1$: $U(t_2,t_1)$ propagates forward in time
$t_2 < t_1$: — " — backward — " —

properties: $U^\dagger(t_2,t_1) = U(t_1,t_2) = U^{-1}(t_2,t_1)$ (U unitarity)
$U(t_3,t_2)\,U(t_2,t_1) = U(t_3,t_1)$
$U(t_1,t_1) = \mathbb{1}$

→ Consider: $\boxed{H(t) = H_0 + \delta H(t)}$

exactly solvable & time-independent (e.g. free particle, harmonic oscillator) "unperturbed" system

"small" time-dependent contribution to be treated perturbatively

Interaction picture:

$U_0(t_2,t_1) = e^{-iH_0(t_2-t_1)}$ → Time-evolution operator of the unperturbed system.

States: $|\psi,t\rangle_I \equiv U_0^+(t,t_0)\,|\psi,t\rangle_S$ ← Schrödinger picture state

$= U_0(t_0,t)\,|\psi,t\rangle_S$ → $|\psi,t_0\rangle_I = |\psi,t_0\rangle_S$, t_0 arbitrary reference time

⇝ Time evolution of the interaction picture state $|\psi,t\rangle_I$ due to H_0 has been eliminated. They contain only the time-evolution coming from $\delta H(t)$

Operators: $A_I(t) = U_0^+(t,t_0)\,A_S(t)\,U_0(t,t_0)$

$= U_0(t_0,t)\,A_S(t)\,U_0(t,t_0)$ ⟶ $A_I(t_0) = A_S(t_0)$

⇝ Interaction picture operators contain time-evolution of the unperturbed H_0.

Recall: S-matrix element for 1 particle scattering in the Schrödinger picture

$S_{fi} = \int d^3\vec{x}\; \psi^*_{final}(t_f,\vec{x})\,\psi^{(+)}_{in}(t_f,\vec{x})$ — With complete $H(t)$ time-evolved in-state.

$= {}_S\langle \psi_f, t_f | \psi^{(+)}_{in}, t_f\rangle_S$

$= {}_S\langle \psi_f, t_f | U^0(t_f,t_i) | \psi_{in}, t_i\rangle_S$

$+ (-i)\int_{t_i}^{t_f} dt\; {}_S\langle \psi, t_f | U_0(t_f,t)\,\delta H_S(t)\,U_0(t,t_i) | \psi_{in}, t_i\rangle_S$

$+ (-i)^2 \int_{t_i}^{t_f} dt_2 \int_{t_i}^{t_2} dt_1\; {}_S\langle \psi, t_f | U_0(t_f,t_2)\,\delta H_S(t_2)\,U_0(t_2,t_1)\,\delta H_S(t_1)\,U_0(t_1,t_i) | \psi_{in}, t_i\rangle_S$

$+ \dots$

$t_i \to -\infty$: $|\psi_{in}, t_i\rangle$
$t_f \to +\infty$: $|\psi_{out}, t_f\rangle$
$\Big\}$ are solutions of the unperturbed problem with $H = H_0$

$\Rightarrow |\psi_f, t_f\rangle_S = U_0(t_f,t_i)\,|\psi_f, t_i\rangle_S$

$$= {}_s\langle \psi_f, t_i | \psi_{in}, t_i \rangle_s$$

$$+ (-i) \int_{t_i}^{t_f} dt \; {}_s\langle \psi, t_i | U_0(t_i, t)\, \delta H_S(t)\, U_0(t, t_i) | \psi_{in}, t_i \rangle_s$$

$$+ (-i)^2 \int_{t_i}^{t_f} dt_2 \int_{t_i}^{t_2} dt_1 \; {}_s\langle \psi, t_i | U_0(t_i, t_2)\, \delta H_S(t_2)\, U_0(t_2, t_1)\, \delta H_S(t_1)\, U_0(t_1, t_i) | \psi_{in}, t_i \rangle_s$$

$$+ \dots$$

↳ We rewrite the S-matrix element in the interaction picture.

"0" for unperturbed asymptotic state

Set $t_0 = t_i$:
$$|\psi_i, t_i\rangle_I = |\psi_i, t_0\rangle_S =: |\psi_{in}^0\rangle$$

$$|\psi_f, t_i\rangle_I = |\psi_f, t_0\rangle_S =: |\psi_f^0\rangle$$

$$\delta H_I(t) = U_0(t_0, t)\, \delta H_S(t)\, U_0(t, t_0)$$

$$U_0(t_n, t_{n-1}) = U_0(t_n, t_0)\, U_0(t_0, t_{n-1})$$

$$\Rightarrow S_{fi} = \langle \psi_f^0 | \psi_{in}^0 \rangle$$

$$+ (-i) \int_{t_i}^{t_f} dt \, \langle \psi_f^0 | \delta H_I(t) | \psi_{in}^0 \rangle$$

$$+ (-i)^2 \int_{t_i}^{t_f} dt_2 \int_{t_i}^{t_2} dt_1 \, \langle \psi_f^0 | \delta H_I(t_2)\, \delta H_I(t_1) | \psi_{in}^0 \rangle + \dots$$

↳ We can rewrite this expression in a very compact for by introducing the time ordering operator T :

$A(t)$, $B(t)$ time-dependent operators :

$$T\, A(t_2) B(t_1) \equiv \Theta(t_2 - t_1)\, A(t_2) B(t_1) + \Theta(t_1 - t_2)\, B(t_1) A(t_2)$$

↳
$$\boxed{S_{fi} = \langle \psi_f^0 | \, T \exp\left\{ -i \int_{t_i}^{t_f} dt \, \delta H_I(t) \right\} | \psi_{in}^0 \rangle}$$

Time ordering operator

At this point we can also set $t_0 = 0$ since it is arbitrary anyway.

Application: System with a small periodic perturbation

$$H = H_0 + \underbrace{H_1 e^{-i\omega t}}_{\delta H(t)} \quad , \omega > 0$$

→ We will reconsider this case when we treat radiation transitions of the H-atom.

Born approximation for S-matrix element: (only transition term) $t_0 = 0$

$$S_{fi}^{Born} = -i \int_{t_i}^{t_f} dt \, \langle f(t=0) | U_0(0,t) \, H_1 e^{-i\omega t} \, U_0(t,0) | in(t=0) \rangle$$

$$= -i \langle f(t=0) | H_1 | in(t=0) \rangle \int_{t_i}^{t_f} dt \, \underbrace{e^{iE_f t} \, e^{-i\omega t} \, e^{-iE_{in} t}}_{\to \, e^{+i(E_f - E_i - \omega)}}$$

$$\xrightarrow{t_{f,i} \to \pm\infty} \; -i \langle f(t=0) | H_1 | in(t=0) \rangle \; 2\pi \, \delta(E_f - E_i - \omega)$$

We see: Periodic oscillation $\sim e^{-i\omega t}$ corresponds to interaction that feeds energy ω into the system.

Periodic oscillation $\sim e^{+i\omega t}$ corresponds to interaction that removes energy ω out of the system.

↳ More later when we deal with interactions of the H-atom with real photons.