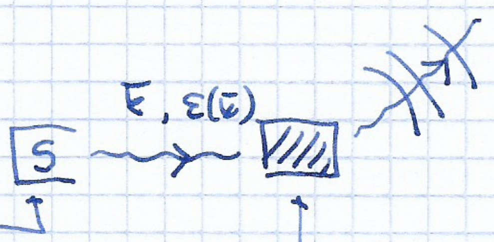
V SCATTERING THEORY

§ 1. INTRODUCTION

Basic setup

D ← detector of scattered particles p'
$\bar{k}' = (\bar{p}', \sigma', \text{etc.})$
with energy $\varepsilon'(\bar{k}')$



source of particles p
$\bar{k} = (\bar{p}, \sigma, \text{etc.})$
with energy $\varepsilon(\bar{k})$

target X $\{\bar{K}, E(\bar{K})\}$
modified to
X' $\{\bar{K}', E'(\bar{K}')\}$

Reaction scheme

$$\boxed{\begin{array}{ccccccc} p & + & X & \longrightarrow & p' & + & X' \\ \updownarrow & & \updownarrow & & \updownarrow & & \updownarrow \\ \bar{k}, \varepsilon(\bar{k}) & & \bar{K}, E(\bar{K}) & & \bar{k}', \varepsilon'(\bar{k}') & & \bar{K}', E'(\bar{K}') \end{array}}$$

note: •) $p \neq p'$ e.g. X-ray $p = h\nu$, $p' = e$

••) elastic – energy of p conserved e.g. X ray on static atoms, inelastic – e.g. neutron on phonons.

> The accessible information on scattering process is stored in the distribution $J(\varepsilon'(\bar{k}'), \bar{k}')$ of scattered particles monitored by a detector

→ Target properties $E(\bar{K})$ deduced.

Energy - momentum conservation law

$$\boxed{\begin{aligned} \bar{k} + \bar{K} &= \bar{k}' + \bar{K}' \\ \varepsilon(\bar{k}) + E(\bar{K}) &= \varepsilon'(\bar{k}') + E'(\bar{K}') \end{aligned}}$$

e.g. A resonant peak in $P(\varepsilon'(\bar{k}), \bar{k})$ signals the existence of an internal structure of momentum $\boxed{\Delta \bar{K} = \bar{K}' - \bar{K} = \bar{k} - \bar{k}'}$ and frequency/energy $\boxed{\Delta E = E' - E = \varepsilon - \varepsilon'}$

Types of scattering experiments

→ Elastic scattering off immobile target

$$\Delta E = -\Delta \varepsilon = 0$$

(heavy target) infinite mass

e.g. crystallography

→ Elastic scattering off mobile target

$$\Delta E = -\Delta \varepsilon = 0$$

e.g. Rutherford scattering

→ Inelastic scattering

energy exchange possible $\Delta E = -\Delta \varepsilon \neq 0$

e.g. quarks in hadronic particles

→ Rearrangement scattering

reaction of participating targets $N_1 + N_2 \to N_1' + N_2' + \ldots$

elastic $N_1 + N_2 \to N_1 + N_2$

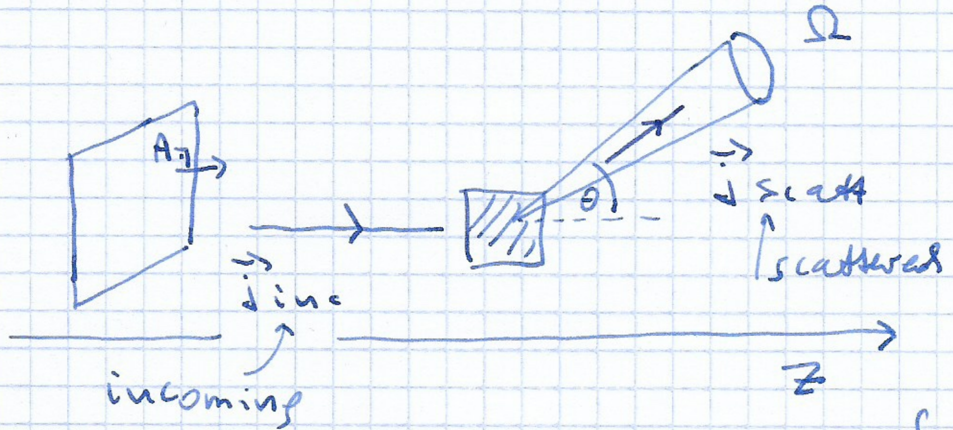
particle production $N_1 + N_2 \to N_1 + N_2 + N_3$

→ Resonant scattering

formation and subsequent decay of unstable particles

§ 2. CROSS SECTION

Differential cross section



detector records number of particles scattered into a solid angle Ω

angular current density
$\vec{j}_{scatt}(\theta,\varphi)$

$\int_A dx\,dy\; j_{inc}(x,y) =$ number of particles per time through area A

$\int_\Omega \sin\theta\, d\theta\, d\varphi\; j_{scatt}(\theta,\varphi) =$

$=$ number of particles per time in cone Ω

dimension $\left[\vec{j}_{inc}\right] = \left[\frac{\text{number of particles}}{\text{area} \times \text{time}}\right]$

dimension $\left[\vec{j}_{scatt}\right] = \left[\frac{\text{number of particles}}{\text{angle} \times \text{time}}\right]$

Df. Differential cross-section $d\sigma$

$$\boxed{\vec{j}_{scatt} \cdot d\vec{\Omega} = \vec{j}_{inc} \cdot d\vec{\sigma}}$$

or

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\vec{j}_{scatt,\hat{n}}}{\vec{j}_{inc,\hat{n}}}}$$

only "normal" components!

not a derivative!

$$\boxed{\left[\frac{d\sigma}{d\Omega}\right] = \left[\text{area}\right]}$$

Df. Total cross-section

$$\boxed{\sigma = \int_{4\pi} d\Omega\, \frac{d\sigma}{d\Omega} = \int_{4\pi} d\sigma}$$

E.g.

visible light	$1cm^2 = 10^{-4}m^2$
x-ray	$1Å^2 = 10^{-20}m^2$
neutron on nuclei	$1b^2 = 10^{-28}m^2$

"The geometric area of individual scattering centers"

§3. GENERAL THEORY – LIPPMAN-SCHWINGER

→ ~~elasti~~ elastic scattering on immobile targets

→ potential scattering, $\underset{\text{target}}{V(\vec{r})} \in \mathbb{R}$

> **Basic problem:** obtain the wave function of scattered particles in such a way that boundary conditions corresponding to an incoming particle beam are imposed

Typically, an incident particle in state $|\phi\rangle$ is scattered by the potential $\hat{V}$ in a scattered state $|\psi_s\rangle$.

→ We assume that $\hat{H}_0 |\phi\rangle = E|\phi\rangle \quad E \in \mathbb{R}$

scattering, continuum states

usually $\hat{H}_0 = \dfrac{\hat{\vec{p}}^2}{2m}$

and then $\phi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \phi \rangle = \dfrac{1}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}$ not normalized

$\vec{p} = \hbar \vec{k}$

→ The scattering potential (target) is "localized"

$\lim_{r\to\infty} V(r) = 0$ sufficiently fast

We need to solve

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle$$

using $\hat{H}_0 |\phi\rangle = E|\phi\rangle$

The same energy → elastic scattering

Lippman Schwinger equation

Df. Scattering state

$$|\psi_s\rangle = |\psi\rangle - |\phi\rangle$$

We note

$$(E - \hat{H}_0)|\psi\rangle = \hat{V}|\psi\rangle$$

$$|\psi\rangle = |\psi_s\rangle + |\phi\rangle$$

$$(E - \hat{H}_0)|\psi_s\rangle + \underbrace{(E - \hat{H}_0)|\phi\rangle}_{=0} = \hat{V}|\psi\rangle$$

$$(E - \hat{H}_0)|\psi_s\rangle = \hat{V}|\psi\rangle \qquad / \ (E - \hat{H}_0)^{-1}$$

$$|\psi_s\rangle = (E - \hat{H}_0)^{-1}\hat{V}|\psi\rangle$$

$$\boxed{|\psi\rangle = |\phi\rangle + (E - \hat{H}_0)^{-1}\hat{V}|\psi\rangle}$$

Lippman-Schwinger equation, equivalent to Schrödinger equation

$$(\hat{H}_0 + V)|\psi\rangle = E|\psi\rangle$$

More suitable to iterative solution.

Formal, implicit solution by recursive means

§4. GREEN FUNCTION & LIPPMAN-SCHWINGER

$$|\psi\rangle = |\phi\rangle + \frac{\hat{V}}{E - \hat{H}_0}|\psi\rangle$$

Problem: $\frac{\hat{V}}{E - \hat{H}_0}$ - does not exist in general,

e.g. if E is eigen value of $\hat{H}_0$!

We avoid this problem by a trick $\boxed{E \to E^+ = E + i\eta, \quad \eta \to 0^+}$

or $E^+ = E + i0^+$

The resolvent $\boxed{\frac{1}{E^+ - \hat{H}_0} =: \hat{G}_0^+(E)}$

is well defined

due to the reality of the spectrum $\hat{H}_0$.

Lippman-Schwinger equation reads

$$\boxed{|\psi\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\psi\rangle}$$

The formal solution

$$(1 - \hat{G}_0^+(E)\,\hat{V})\,|\psi\rangle = |\phi\rangle$$

$$\boxed{|\psi\rangle = (1 - \hat{G}_0^+(E)\,\hat{V})^{-1}|\phi\rangle}$$

What is the meaning of the trick
$E \to E^+ = E + i0^+$?

<u>Time dependent formulation of LP equation</u>

Consider time dependent Schrödinger equation

$$\boxed{\left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0\right)|\Psi(t)\rangle = \hat{V}\,|\Psi(t)\rangle}$$

Boundary condition (appropriate in scattering problems) is that in a remote past the particle was free, i.e.

as $t \to -\infty$ $\qquad \left(i\hbar \frac{\partial}{\partial t} + \hat{H}_0\right)|\Psi(t)\rangle = 0$

[Indeed, ok for short range $V(r)$]

This boundary condition is accomplished by adiabatic turning on of the potential

$$\boxed{\hat{V} \longrightarrow \lim_{\varepsilon \to 0^+} \hat{V} e^{t\varepsilon}} \leftarrow \hat{V}(t)$$

We solve the Schrödinger equation by introducing the <u>Green's operator</u> $\hat{G}_0^+(t,t')$ satisfying

$$\boxed{\left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0\right)\hat{G}_0^+(t,t') = \delta(t-t')} \quad (*)$$

The <u>causality</u> principle requires that the interaction of a particle at t' has an effect only for $t > t'$!

→ we define <u>retarded</u> boundary condition

where $\boxed{\hat{G}_0^+(t,t') = 0 \quad \text{for} \quad t < t'}$

Then the solution of $(*)$ is

$$\boxed{\hat{G}_0^+(t,t') = -\frac{i}{\hbar}\,\theta(t-t')\,e^{-\frac{i\hat{H}_0(t-t')}{\hbar}}}$$

Indeed, with

$$i\hbar\frac{\partial}{\partial t}\left[-\frac{i}{\hbar}\,\theta(t-t')\right] = \delta(t-t')$$

we can obtain $(*)$.

Solution of the full problem is

$$\boxed{|\Psi^+(t)\rangle = |\Phi(t)\rangle + \int_{-\infty}^{\infty} \hat{G}_0^+(t,t')\,\hat{V}(t')|\Psi^+(t')\rangle\,dt'}$$

where $\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_0\right)|\Phi(t)\rangle = 0$

Indeed,

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_0\right)|\Psi^+(t)\rangle = \overbrace{\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_0\right)|\Phi(t)\rangle}^{=0} +$$

$$+ \int_{-\infty}^{\infty} \underbrace{\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_0\right)\hat{G}_0^+(t,t')}_{\delta(t,t')}\,\hat{V}\,|\Psi^+(t')\rangle\,dt' =$$

$$= \hat{V}(t)|\Psi^+(t)\rangle$$

$\square$

Limiting ourselves to stationary states

$$|\Phi(t)\rangle = e^{-i\frac{Et}{\hbar}}\,|\phi\rangle$$

$$|\Psi(t)\rangle = e^{-i\frac{Et}{\hbar}}\,|\psi\rangle$$

[E is not changed when $\hat{V}$ is switched on]

$$\cancel{e^{-i\frac{Et}{\hbar}}}\,|\psi\rangle = \cancel{e^{-i\frac{Et}{\hbar}}}\,|\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt'\,\theta(t-t')\,e^{\frac{-i\hat{H}_0(t-t')}{\hbar}}\,\hat{V}(t')\,e^{-i\frac{Et'}{\hbar}}|\psi\rangle$$

$\cancel{e^{-i\frac{Et}{\hbar}}}\,|\psi\rangle$

At $t=0$

$$|\psi\rangle = |\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{0} dt'\,e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\hbar\varepsilon)t'}\,\hat{V}\,|\psi\rangle =$$

$$= |\phi\rangle - \frac{i}{\hbar}\,\frac{1 - \lim_{t'\to-\infty} e^{\frac{i}{\hbar}(\hat{H}_0 - E - i\hbar\varepsilon)t'}}{\frac{i}{\hbar}(\hat{H}_0 - E - i\underbrace{\hbar\varepsilon}_{\eta})}\,\hat{V}\,|\psi\rangle$$

$$|\psi\rangle = |\phi\rangle + \frac{\hat{V}}{E + i\eta - \hat{H}_0}\,|\psi\rangle$$

→ LP equation

⇒ $\boxed{\text{The } \eta \text{ trick } E \to E^+ = E + i\eta \text{ corresponds to the retarded boundary condition}}$

Mathematically, one can use advanced boundary condition, $E \to E^- = E - i\eta$, unphysical but formally important too.

with

$$\boxed{\begin{aligned} |\Psi^-(t)\rangle &= |\Phi^-(t)\rangle + \int_{-\infty}^{\infty} dt'\,\hat{G}_0^-(t,t')\,\hat{V}(t')\,|\Psi^-(t')\rangle \\ \hat{G}_0^-(t,t') &= \frac{i}{\hbar}\,\theta(t'-t)\,e^{-\frac{i}{\hbar}\hat{H}_0(t-t')} \end{aligned}}$$

§5. FORMAL SOLUTION OF LIPPMAN–SCHWINGER EQUATION

The scattered state $|\psi_s\rangle = |\psi\rangle - |\phi\rangle$

L-S-Eq.

$$|\psi\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\psi\rangle$$

solve recursively

$$|\psi^0\rangle = |\phi\rangle$$

$$|\psi^1\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle$$

$$|\psi^2\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,\hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle$$

$$\vdots$$

$$\boxed{|\psi\rangle = |\phi\rangle + \sum_{n=1}^{\infty}\left(\hat{G}_0^+(E)\,\hat{V}\right)^n|\phi\rangle}$$

It is like a geometric series which "converges" to

$$\boxed{|\psi\rangle = \frac{1}{1-\hat{G}_0(E)\,\hat{V}}\,|\phi\rangle}$$

$(1-A)^{-1} = 1 + A + A^2 + \dots$

For the scattered state

$$|\psi_s\rangle = \hat{G}_0^+\,\hat{V}\,|\phi\rangle + \left(\hat{G}_0^+\,\hat{V}\right)^2|\phi\rangle + \dots =$$

$$= \hat{G}_0\,\hat{V}\left(1 + \hat{G}_0\,\hat{V} + (\hat{G}_0\,\hat{V})^2 + \dots\right)|\phi\rangle =$$

$$= \hat{G}_0\,\hat{V}\left(1 - \hat{G}_0\,\hat{V}\right)^{-1}|\phi\rangle$$

We introduce <u>T-matrix</u>

$$\boxed{\hat{T}(E) \equiv \hat{V}\,(1 - \hat{G}_0^+(E)\,\hat{V})^{-1}}$$

or equivalently $\boxed{\hat{T}(E) = (1 - \hat{V}\,\hat{G}_0(E))^{-1}\,\hat{V}}$

Indeed, by multiplying by $(1 - \hat{V}\hat{G}_0^+)$ from the left and by $(1 - \hat{G}_0^+\hat{V})$ from the right

1) $(1 - \hat{V}\hat{G}_0^+)\,\hat{T}\,(1 - \hat{G}_0^+\hat{V}) = (1 - \hat{V}\hat{G}_0^+)\,\hat{V}\,\overbrace{(1 - \hat{G}_0^+\hat{V})^{-1}(1 - \hat{G}_0^+\hat{V})}^{1}$

$\qquad\qquad \parallel$

2) $(1 - \hat{V}\hat{G}_0^+)\,\hat{T}\,(1 - \hat{G}_0^+\hat{V}) = \underbrace{(1 - \hat{V}\hat{G}_0^+)(1 - \hat{V}\hat{G}_0^+)^{-1}}_{1}\,\hat{V}\,(1 - \hat{G}_0^+\hat{V})$

$$\rightarrow \quad \hat{V} - \hat{V}\hat{G}_0^+\hat{V} = \hat{V} - \hat{V}\hat{G}_0^+\hat{V}$$

$\square$

<u>Expanding T-matrix</u>

$$\boxed{\hat{T}(E) = \hat{V} + \hat{V}\hat{G}_0^+(E)\hat{V} + \hat{V}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V} + \cdots}$$

T-matrix represents a series of multiple scatterings on potential $\hat{V}$

$$\boxed{|\psi_s\rangle = \hat{G}_0(E)\,\hat{T}(E)\,|\phi\rangle}$$

effective "scattering potential"

L-P equation for the wave function

$$\psi(r) = \langle r | \psi \rangle \quad , \quad \varphi(r) = \langle r | \varphi \rangle$$

$$\boxed{\psi(r) = \varphi(r) + \int dr' \, G_0^+(r, r'; E) \, V(r') \, \psi(r')}$$

where we used

$$1 = \int dr' \, |r'\rangle\langle r'|$$

and

$$\boxed{G_0^+(r, r'; E) = \langle r | \hat{G}_0^+(E) | r' \rangle}$$

is the Green's function

propagator from $|r'\rangle$ to $|r\rangle$

In terms of the infinite series

$$\boxed{\begin{aligned} \psi(r) = \varphi(r) &+ \int dr' \, G_0^+(r, r'; E) \, V(r') \, \varphi(r') + \\ &+ \int dr' \int dr'' \, G_0^+(r, r'; E) \, V(r') \, G(r', r'', E) \, V(r'') \, \varphi(r'') + \\ &+ \dots \end{aligned}}$$

Born series

$$\boxed{\begin{aligned} T(r, r', E) = {} & V(r) \, \delta(r - r') + V(r) \, G_0^+(r, r'; E) \, V(r') + \\ &+ \int dr'' \, V(r) \, G_0^+(r, r', E) \, V(r') \, G_0^+(r', r'', E) \, V(r'') + \dots \end{aligned}}$$

$$\boxed{T(r, r'; E) = \langle r | \hat{T}^+(E) | r' \rangle}$$