III.5 Formal scattering theory: Lippman-Schwinger equation

In the following we will discuss a more general approach to scattering theory which encompasses single-particle scattering at a given external potential as well as two- (or many) body scattering.

consider Hamiltonian with scattering term $\hat{V}$ (external potential or two-particle interaction ...)

$$(151) \qquad \hat{H} = \hat{H}_0 + \hat{V} \underbrace{e^{-\varepsilon|t|/\hbar}} \qquad \varepsilon > 0$$

asymptotic switch on/off of interaction $\hat{V}$
for $|t| \to \infty$ $\hat{H} = \hat{H}_0$ later $\varepsilon \to 0$

consider interaction picture $t=0$ Int. pict. = Schrödinger

$$(152) \qquad |\psi_I(t)\rangle = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle$$

and $\hat{V}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{V} e^{-i\hat{H}_0 t/\hbar}$ where $\varepsilon \to 0$

$$(153) \Rightarrow \qquad i\hbar \frac{d}{dt} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle$$

formal solution

$$(154) \qquad |\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar} \int_{t_0}^{t} d\tau \, \hat{V}_I(\tau) \, |\psi_I(\tau)\rangle$$

noting that for $t_0 \to \pm\infty$ due to the term $e^{-\varepsilon|t|/\hbar}$

$$\hat{V}_I(t_0) \to 0 \qquad \text{with } t_0 = \pm\infty$$

i.e.

(155) $$|\psi_I(t \to \pm\infty)\rangle = |\phi^{(\pm)}\rangle$$ free solutions of Schrödinger equation

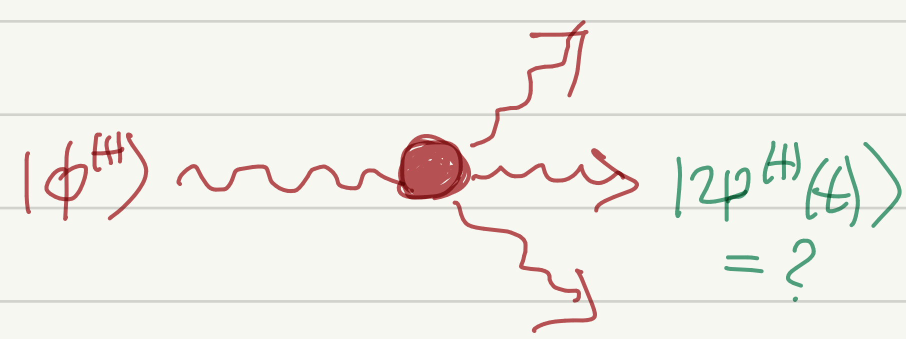
thus depending on $t_0 = +\infty$ or $t_0 = -\infty$

(156) $$\boxed{|\psi_I^{(\pm)}(t)\rangle = |\phi^{(\pm)}\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} d\tau\, \hat{V}_I(\tau)\,|\psi_I^{(\pm)}(\tau)\rangle}$$

- $|\psi_I^{(+)}(t)\rangle$ is called <u>retarded solution</u>

  here the solution ("in" state) for $t \to -\infty$ is known and a free solution

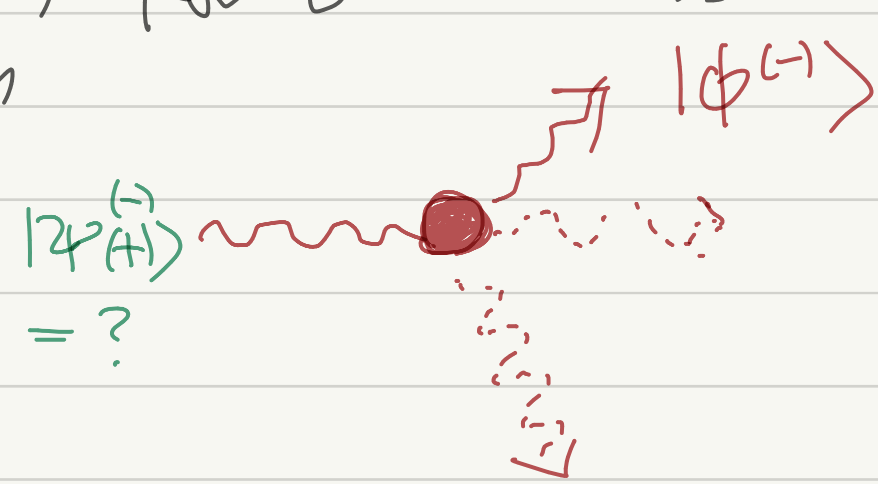
  $$|\psi_I^{(+)}(t \to -\infty)\rangle = |\phi^{(+)}\rangle$$



- $|\psi_I^{(-)}(t)\rangle$ is called <u>advanced solution</u>

  here the solution ("out" state) for $t \to +\infty$ is known and a free solution

  $$|\psi_I^{(-)}(t \to +\infty)\rangle = |\phi^{(-)}\rangle$$



choosing that int. picture = Schrödinger picture at $t=0$

i.e.

$$\underset{\text{interaction p.}}{|\psi_I^{(\pm)}(0)\rangle} = \underset{\text{Schrödinger p.}}{|\psi^{(\pm)}(0)\rangle} \equiv |\psi^{(\pm)}\rangle \tag{157}$$

and look for <u>energy eigenstates</u>

$$\hat{H}|\psi^{(\pm)}\rangle = E|\psi^{(\pm)}\rangle \tag{158}$$

$$\overset{(156)}{\Rightarrow} |\psi^{(\pm)}\rangle = |\phi^{(\pm)}\rangle - \frac{i}{\hbar}\int_{\mp\infty}^{0} d\tau\, e^{iH_0\tau/\hbar} V(\tau) e^{-iH_0\tau/\hbar} e^{-\varepsilon|\tau|/\hbar} \cdot |\psi_I^{(\pm)}(\tau)\rangle$$

using furthermore

$$|\psi_I^{(\pm)}(\tau)\rangle = e^{i\hat{H}_0\tau/\hbar}|\psi^{(\pm)}(\tau)\rangle$$

$$= e^{i\hat{H}_0\tau/\hbar} e^{-i\hat{H}\tau/\hbar} \underbrace{|\psi^{(\pm)}(0)\rangle}_{=|\psi^{(\pm)}\rangle}$$

With this we finally arrive at

$$|\psi^{(\pm)}\rangle = |\phi^{(\pm)}\rangle - \frac{i}{\hbar}\int_{\mp\infty}^{0} d\tau\, e^{\frac{i\hat{H}_0\tau}{\hbar}} \hat{V} e^{-\varepsilon|\tau|/\hbar} e^{-\frac{i\hat{H}\tau}{\hbar}} |\psi^{(\pm)}\rangle \tag{157}$$

eigenvalue eq. (158)

$\Rightarrow$ integral equation for exact scattering state

$$\boxed{|\psi^{(\pm)}\rangle = |\phi^{(\pm)}\rangle - \frac{i}{\hbar}\int_{\mp\infty}^{0} d\tau\, e^{\frac{i\hat{H}_0\tau}{\hbar}} \hat{V} e^{-\frac{\varepsilon|\tau|}{\hbar}} e^{-\frac{iE\tau}{\hbar}} |\psi^{(\pm)}\rangle} \tag{158}$$

Let us now define

Green's Operator

$$\hat{G}_0^{(\pm)} \equiv -\frac{i}{\hbar}\int_{\mp\infty}^{0} d\tau \, \exp\left\{\frac{i(\hat{H}_0 - E \mp i\varepsilon)\tau}{\hbar}\right\} \tag{159}$$

$\mp i\varepsilon$ is important to avoid singular behaviour

$$\boxed{\hat{G}_0^{(\pm)} = -\frac{1}{\hat{H}_0 - E \mp i\varepsilon}} \tag{160}$$

Green's Operator at energy E

completely determined by eigenspectrum of $\hat{H}_0$!

With (160) we can write the integral equation (158) in the form

$$\boxed{\begin{aligned} |\psi^{(\pm)}\rangle &= |\phi^{(\pm)}\rangle + \hat{G}_0^{(\pm)} \hat{V} |\psi^{(\pm)}\rangle \\ &= |\phi^{(\pm)}\rangle - \frac{1}{\hat{H}_0 - E \mp i\varepsilon} \hat{V} |\psi^{(\pm)}\rangle \end{aligned}} \tag{161}$$

Lippmann-Schwinger equation

This is an equation for a self-consistent calculation of the true scattering state $|\psi^{(\pm)}\rangle$ from the in or out solutions $|\phi^{(\pm)}\rangle$.

Iteration of eq. (161) yields the Born series

$$(162)\quad \boxed{|\psi^{(\pm)}\rangle = \left[\mathbb{1} + \hat{G}_0^{(\pm)}\hat{V} + \hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \dots\right]|\phi^{(\pm)}\rangle}$$

In order to evaluate the Born series we can go to a spatial representation

since H_0 in spatial representation is a differential operator we expect that $G_0 \sim (H_0 - E \pm i\varepsilon)^{-1}$ is an integral operator

$$(163)\quad \hat{G}_0^{(\pm)}|\psi\rangle = \int d^3r \int d^3r' \, |\vec{r}\rangle \underbrace{\langle\vec{r}|\hat{G}_0^{(\pm)}|\vec{r}'\rangle}_{G_0^{(\pm)}(\vec{r},\vec{r}')} \underbrace{\langle\vec{r}'|\psi\rangle}_{\psi(\vec{r}')}$$

i.e.

$$\hat{G}_0^{(\pm)}|\psi\rangle \longleftrightarrow \int d^3r' \, G_0^{(\pm)}(\vec{r},\vec{r}')\,\psi(\vec{r}')$$

now

$$(164)\quad G_0^{(\pm)}(\vec{r},\vec{r}') = \langle\vec{r}|\hat{G}^{(\pm)}|\vec{r}'\rangle$$

$$= \langle\vec{r}|(\hat{H}_0 - E \mp i\varepsilon)^{-1}|\vec{r}'\rangle = ?$$

in spatial representation

$$-(\hat{H}_0 - E \mp i\varepsilon)\, G_0^{(\pm)}(\vec{r},\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')$$

$\mathbb{1}$ in spatial rep.

i.e. spatial representation of $\hat{G}^{(\mp)}$ is the Greens-function of the Helmholtz-equation

(165) $$\boxed{\left(\frac{\hbar^2}{2m}\Delta_{\vec{r}} + E \pm i\varepsilon\right) G_0^{(\pm)}(\vec{r},\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}')}$$

This Greensfunction can easily be calculated by Fourier-transform. From (165) we see

(166) $$G_0^{(\pm)}(\vec{r},\vec{r}') = G_0^{(\pm)}(\vec{r}-\vec{r}') = \frac{1}{(2\pi)^3}\int d^3q \; e^{i\vec{q}\cdot\vec{x}} \, \tilde{G}_0^{(\pm)}(\vec{q})$$

where $\vec{x} \equiv \vec{r}-\vec{r}'$. F-Trafo of (165) yields

$$\left(-\frac{\hbar^2 q^2}{2m} + E \pm i\varepsilon\right)\tilde{G}_0^{(\pm)}(\vec{q}) = 1$$

(167) $$\boxed{\tilde{G}_0^{(\pm)}(\vec{q}) = -\frac{2m}{\hbar^2}\frac{1}{q^2-k^2 \mp i\tilde{\varepsilon}}}$$

(168) where $$\tilde{\varepsilon} = \frac{2m}{\hbar^2}\varepsilon \qquad E = \frac{\hbar^2 k^2}{2m}$$

inverse F-trafo gives

$$G_0^{(\pm)}(\vec{x}) = -\frac{2m}{(2\pi)^3\hbar^2}\int d^3\vec{q} \, \frac{e^{i\vec{q}\vec{x}}}{q^2-k^2 \mp i\tilde{\varepsilon}}$$

$$= -\frac{2m}{(2\pi)^3\hbar^2}\int_0^\infty dq\, q^2 \underbrace{\int_0^\pi d\vartheta\, \sin\vartheta}_{\xi=\cos\vartheta}\ \underbrace{\int_0^{2\pi} d\varphi}_{=2\pi}\ \frac{e^{iqx\cos\vartheta}}{q^2-k^2\mp i\tilde{\varepsilon}}$$

$$= -\frac{2m}{(2\pi)^2\hbar^2}\int_0^\infty dq\, q^2 \int_{-1}^{1} d\xi\, \frac{e^{iqx\xi}}{q^2-k^2\mp i\tilde{\varepsilon}}$$

$$= -\frac{2m}{(2\pi)^2\hbar^2}\int_0^\infty dq\, q\cancel{^2}\,\frac{1}{i\cancel{q}x}\,\frac{e^{iqx}-e^{-iqx}}{q^2-k^2\mp i\tilde{\varepsilon}}$$

$$= -\frac{2m}{4\pi^2 i\hbar}\int_{-\infty}^{\infty} dq\, \frac{q\,e^{iqx}}{q^2-k^2\mp i\tilde{\varepsilon}}$$

<u>residue integration</u>

1st order pole's in complex plane ($\varepsilon \to 0$ i.e. $\tilde{\varepsilon}\to 0$)

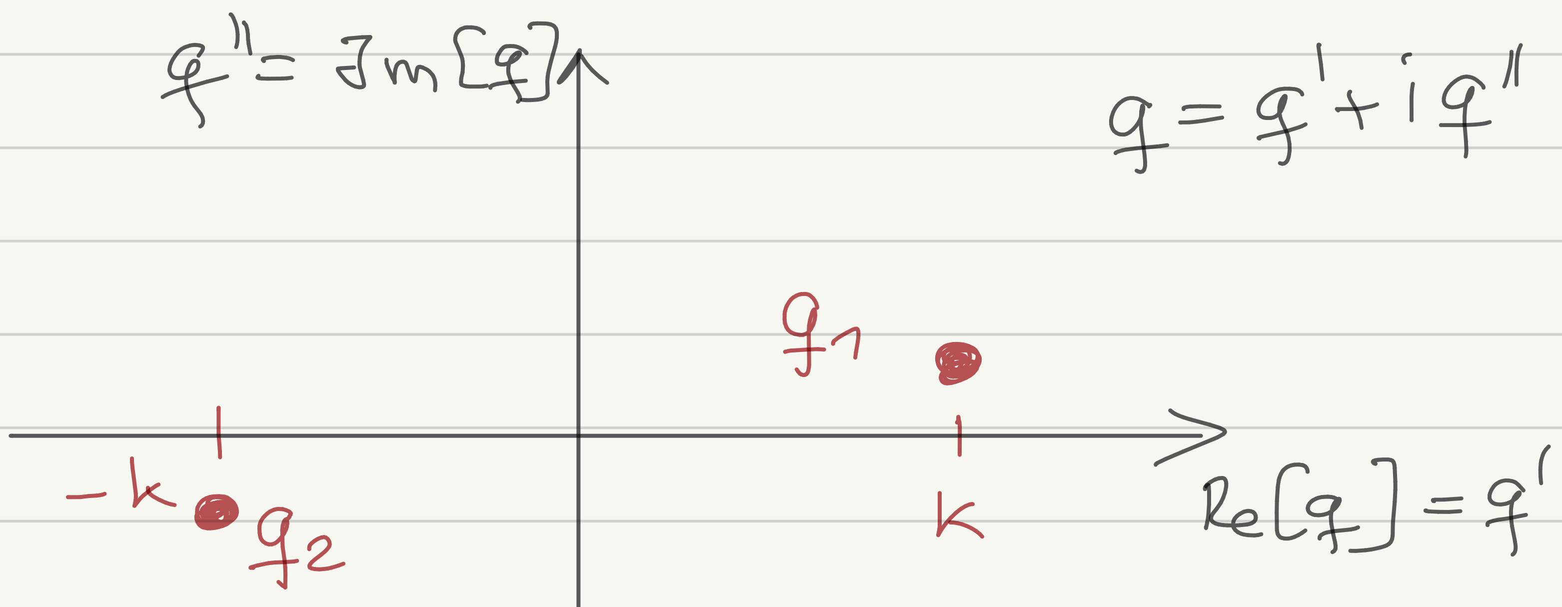
(169) $q^2-k^2-i\tilde{\varepsilon} = (q-k-i\tilde{\tilde{\varepsilon}})(q+k+i\tilde{\tilde{\varepsilon}})$ $\quad(\tilde{\tilde{\varepsilon}}^2\approx 0)$

choose

$\qquad = (q-q_1)(q-q_2)$

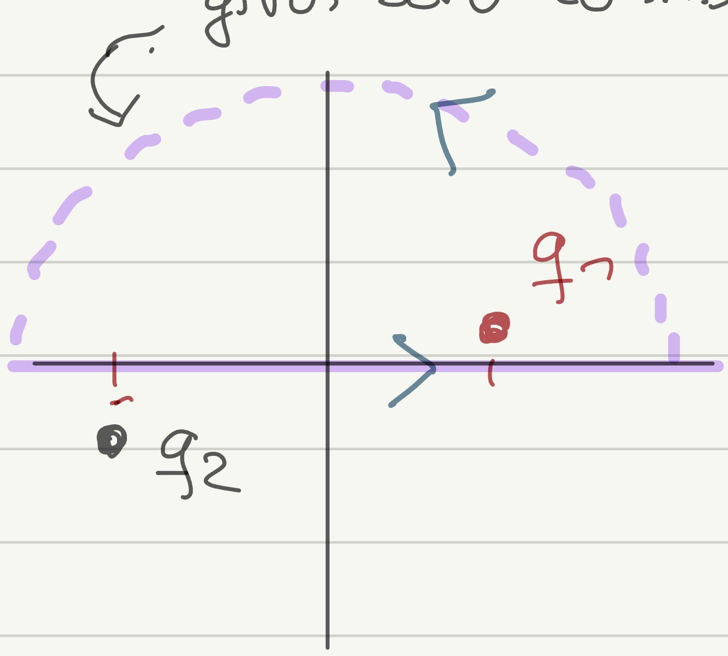
$q_1 = k+i\tilde{\tilde{\varepsilon}}$ $\qquad$ $q_2 = -k-i\tilde{\tilde{\varepsilon}}$

$q = q' + iq''$

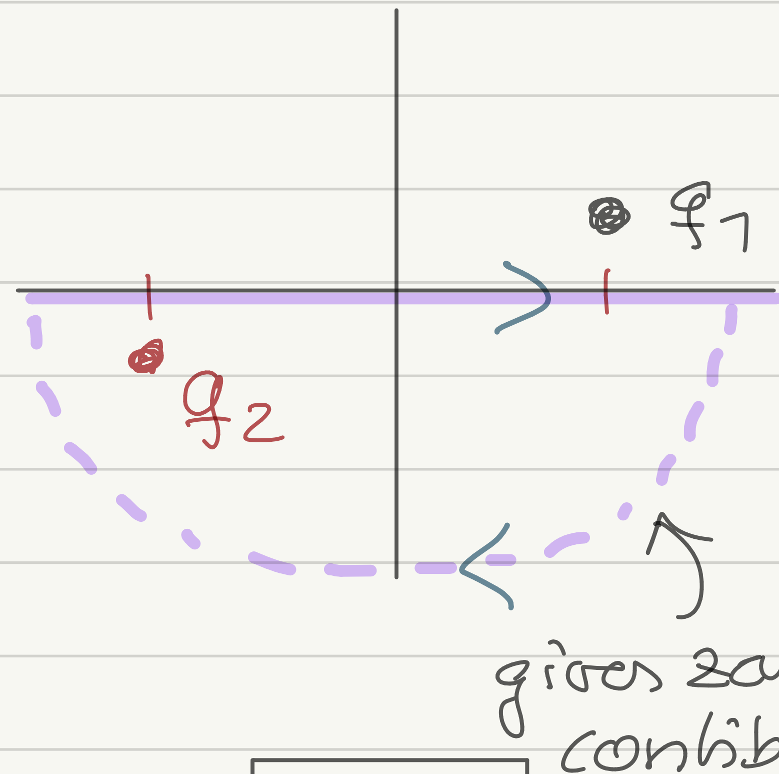


now

(170) $$e^{iqx} = \underbrace{e^{iq'x}}_{\text{bounded}}\ \underbrace{e^{-q''x}}_{\to 0 \text{ for}} \qquad \begin{matrix} x>0 & q''>0 \\ x<0 & q''<0 \end{matrix}$$



$\boxed{x>0}$



$\boxed{x<0}$

(171) $$\int_{-\infty}^{\infty} dq\, \frac{q\, e^{iqx}}{q^2-k^2-i\tilde{\varepsilon}} = 2\pi i \sum_{q_i} \mathrm{Res}\left\{\frac{q\,e^{iqx}}{q^2-k^2-i\tilde{\varepsilon}}\right\}_{q_i}$$

inside integration path

$\underline{x>0|}$

$$= 2\pi \lim_{q\to q_1} (q-q_1)\frac{q\,e^{iqx}}{q^2-k^2-i\tilde{\varepsilon}}$$

$$= \pi i\, e^{ikx}$$

similar for $x<0$

(172) $$\boxed{\begin{aligned} G_0^{(+)}(\vec{x}) &= -\frac{2m}{\hbar^2}\frac{e^{ik|\vec{x}|}}{4\pi|\vec{x}|} \\ G_0^{(-)}(\vec{x}) &= -\frac{2m}{\hbar^2}\frac{e^{-ik|\vec{x}|}}{4\pi|\vec{x}|} \end{aligned}}$$

retarded GF

advanced GF

this then yields the spatial representation of the Lippmann-Schwinger equation

$$\boxed{\psi_k^{(\pm)}(\vec r) = \phi_k^{(\pm)}(\vec r) - \frac{2m}{\hbar^2}\int d^3\vec r\,' \frac{e^{\pm ik|\vec r - \vec r\,'|}}{4\pi|\vec r - \vec r\,'|} V(\vec r\,')\psi_k^{(\pm)}(\vec r\,')}$$

(173)

iteration gives the Born series in spatial representation

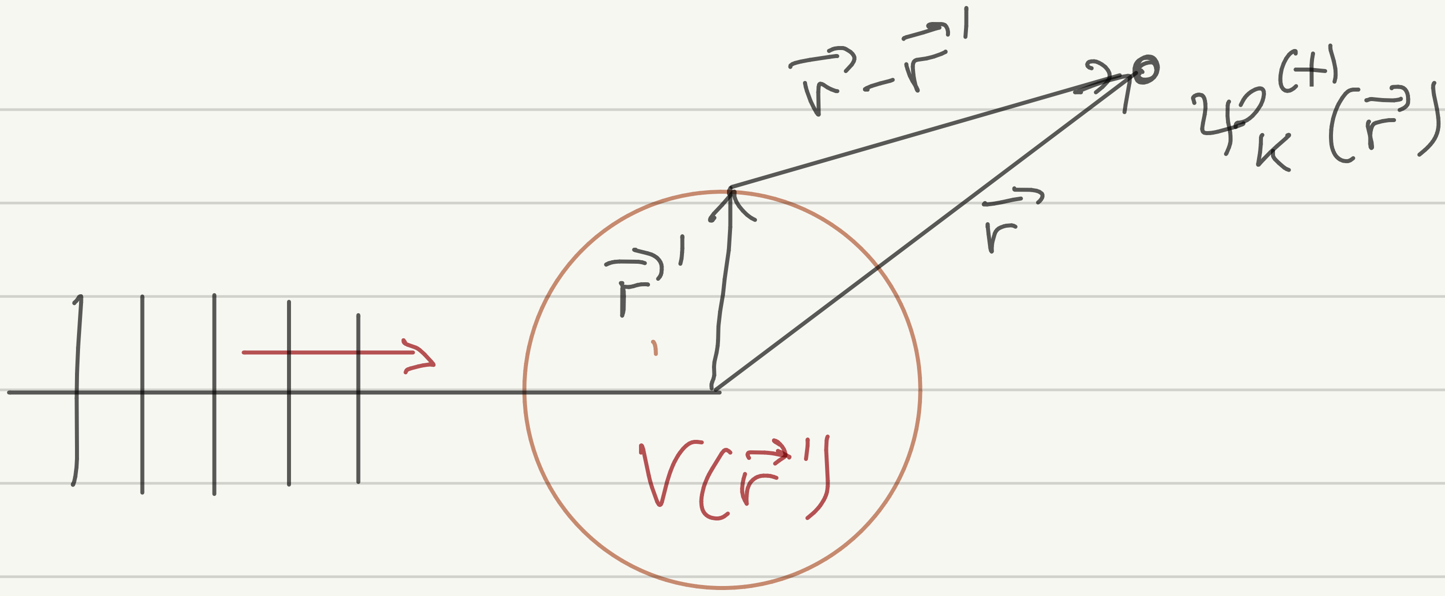
(174)
$$\psi_k^{(\pm)}(\vec r) = \phi_k^{(\pm)}(\vec r) - \frac{2m}{\hbar^2}\int d^3\vec r\,' \frac{e^{\pm ik|\vec r - \vec r\,'|}}{4\pi|\vec r - \vec r\,'|} V(\vec r\,')\phi_k^{(\pm)}(\vec r\,')$$
$$+\left(\frac{2m}{\hbar^2}\right)^2\int d^3r'\int d^3r'' \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|}V(r')\frac{e^{\pm ik|r'-r''|}}{4\pi|r'-r''|}V(r'')\phi_k^{(\pm)}(r'')$$
$$- + \cdots$$

(vector arrows dropped)

What is the connection between $\psi_k^{(\pm)}(\vec r)$ and the scattering amplitude $f_k(\vartheta)$?

(175) $\phi_k^{(+)}(\vec r) = e^{ikz}$

(176) $\psi_k^{(+)}(\vec r) = e^{ikz} - \frac{2m}{\hbar^2}\int d^3 r' \frac{e^{ik|\vec r - \vec r\,'|}}{4\pi|\vec r - \vec r\,'|} V(\vec r\,')\psi_k^{(+)}(\vec r\,')$



large distance from scattering center

$$|\vec{r}-\vec{r}\,'| = \sqrt{(\vec{r}-\vec{r}\,')\cdot(\vec{r}-\vec{r}\,')}$$

$$= \sqrt{r^2 + r'^2 - 2\vec{r}\cdot\vec{r}\,'} \simeq r - \frac{\vec{r}\cdot\vec{r}\,'}{r}$$

(177) $$\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|} \simeq \frac{e^{ikr}}{4\pi r}\, e^{-ik\frac{\vec{r}\cdot\vec{r}\,'}{r}}$$

(178) $$\vec{k}\,' \equiv k\frac{\vec{r}}{r}$$ momentum vector in radial direction from center

$$|\vec{k}\,'| = |\vec{k}| = k$$

(179) $$\boxed{f_k(\vartheta) = -\frac{m}{2\pi\hbar^2}\int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\, V(\vec{r}\,')\, \psi_k^{(+)}(\vec{r}\,')}$$

relation between scattering wavefunction and scattering amplitude

This expression will be particularly useful when we discuss approximate solutions of the scattering problem $\rightarrow$ next section

III.6 T-matrix and Born approximation

If we want to solve the Lippmann-Schwinger equation we face the inconvenience that we have to do this for every input (free) state again. ☹

$$|\psi^{(\pm)}\rangle = |\phi^{(\pm)}\rangle - \frac{1}{\hat{H}_0 - E \mp i\varepsilon}\hat{V}|\psi^{(\pm)}\rangle \tag{180}$$

Can we solve this in a more elegant way? Yes!
Consider again the Born series

$$|\psi_k^{(\pm)}\rangle = \Big[1 + \hat{G}_0^{(\pm)}\hat{V} + \hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \dots\Big]|\phi_k^{(\pm)}\rangle \tag{181}$$

we recognize that the contribution of the scattering potential $\hat{V}$ can be summed up

$$\hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \dots$$

Def: Transfer matrix (at energy $E_k = \frac{\hbar^2 k^2}{2m}$)

$$\boxed{\hat{T}^{(\pm)} \equiv \hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \dots} \tag{182}$$

$$\boxed{|\psi_k^{(\pm)}\rangle = \Big[1 + \hat{G}_0^{(\pm)}\hat{T}^{(\pm)}\Big]|\phi_k^{(\pm)}\rangle} \tag{183}$$

One realizes that $\hat{T}^{(\pm)}$ fulfills the following equation

(184) $$\boxed{\hat{T}^{(\pm)} = \hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{T}^{(\pm)}}$$

Lippmann-Schwinger eq. for T-matrix

In contrast to the Lippmann-Schwinger equation (180) for the state this equation is independent of the initial state!

Rem.: in spatial representation T is non-local

(185) $$T^{(\pm)}(\vec{r},\vec{r}\,') = V(\vec{r})\,\delta^{(3)}(\vec{r}-\vec{r}\,') + \int d^3r''\, V(\vec{r})\, G_0^{(\pm)}(\vec{r}-\vec{r}\,'')\, T^{(\pm)}(\vec{r}\,'',\vec{r}\,')$$

Born approximation

We will now derive an approximate solution of the scattering problem, called Born approximation

Born series for T-matrix

$$\hat{T}^{(\pm)} = \hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V} + \hat{V}\hat{G}_0^{(\pm)}\hat{V}\hat{G}_0^{(\pm)}\hat{V} + \dots$$

$$= \hat{V}\sum_{n=0}^{\infty}\left(\hat{G}_0^{(\pm)}\hat{V}\right)^n$$

if $\hat{G}_0^{(\pm)}\hat{V}$ "small" $\rightarrow$ truncation of series

First-order Born approximation

(186) $$\boxed{\hat{T}^{(\pm)} = \hat{V}}$$

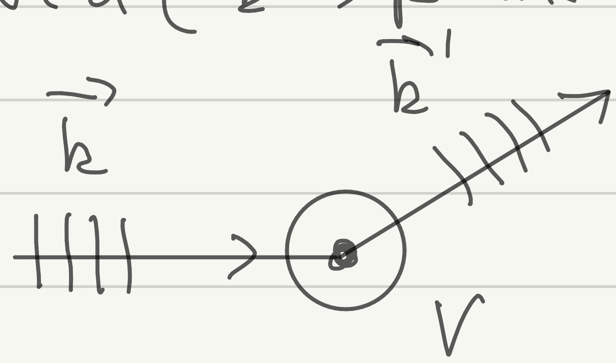
in spatial representation $T^{(\pm)}(\vec{r},\vec{r}\,') = V(\vec{r})\,\delta^{(3)}(\vec{r}-\vec{r}\,')$
local!

(187) $$\boxed{|\psi_k^{(\pm)}\rangle^{(1)} = |\phi_k^{(\pm)}\rangle + \hat{G}_0^{(\pm)}\hat{V}|\phi_k^{(\pm)}\rangle}$$

Now we can use eq. (179) to find the expression for the scattering amplitude in lowest-order Born approximation

(188) $$\boxed{f_k^{(1)}(\vartheta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d^3r'\, e^{-i\vec{k}\,'\cdot\vec{r}\,'}\,V(\vec{r}\,')\,\underbrace{e^{i\vec{k}\cdot\vec{r}\,'}}_{\phi_k^{(\pm)}(\vec{r}\,')}}$$

we see that $f_k^{(1)}(\vartheta,\varphi)$
matrix element of the scattering potential (interaction hamiltonian) between incoming ($\vec{k}$) and scattered ($\vec{k}\,'$) plane wave



(189) $$\boxed{f_k^{(1)}(\vartheta,\varphi) = -\frac{m}{2\pi\hbar^3}(2\pi)^{3/2}\langle\vec{k}|\hat{V}|\vec{k}'\rangle}$$

• Let us discuss this for a central potential $V(\vec{r}) = V(r)$

$$\vec{q} \equiv \vec{k} - \vec{k}' \qquad \tilde{\vartheta} \equiv \sphericalangle(\vec{k}', \vec{r}')$$

$$f_k^{(1)}(\vartheta) = -\frac{m}{2\pi\hbar^2}\int d^3r'\, e^{iqr'\underbrace{\cos\tilde{\vartheta}}_{\xi}}\, V(r')$$

$$= -\frac{m}{\hbar^2}\int_0^\infty dr'\, r'^2 \int_{-1}^{1} d\xi\, e^{iqr'\xi}\, V(r')$$

$$= -\frac{m}{\hbar^2}\int_0^\infty dr'\, r'^2\, \frac{2\sin qr'}{qr'}\, V(r')$$

(190) $$\boxed{f_k^{(1)}(\vartheta) = -\frac{2m}{\hbar^2}\int_0^\infty dr'\, r' V(r') \sin qr'}$$

scattering amplitude of central potential in first-order Born approximation

Now $$q = \sqrt{\vec{q}\cdot\vec{q}} = \sqrt{(\vec{k}-\vec{k}')\cdot(\vec{k}-\vec{k}')}$$

$$= \sqrt{k^2 + k'^2 - 2kk'\cos\vartheta} = k\sqrt{2(1-\cos\vartheta)}$$

(191) $$\boxed{q = 2k\sin\frac{\vartheta}{2}}$$

Example: Screened Coulomb potential

$$V(r) = -\frac{Ze^2}{r}\exp(-r/a)$$

Yukawa, or Thomas-Fermi

$$f_k^{(1)}(\vartheta) = \frac{2mZe^2}{\hbar^2 q}\int_0^\infty dr'\, e^{-r'/a}\sin qr'$$

$$= \dots = \frac{2mZe^2}{\hbar^2 \cancel{q}}\,\frac{\cancel{q}}{q^2+(1/a)^2}$$

with (191):

$$f_k^{(1)}(\vartheta) = \frac{2mZe^2}{\hbar^2}\,\frac{1}{\left(2k\sin\frac{\vartheta}{2}\right)^2+\left(\frac{1}{a}\right)^2}$$

this gives the differential cross section

$$\frac{d\sigma_k^{(1)}}{d\Omega} = \frac{\left(2mZe^2/\hbar^2\right)^2}{\left[\left(2k\sin\frac{\vartheta}{2}\right)^2+\left(\frac{1}{a}\right)^2\right]^2}$$

$$\Big\downarrow\ a\to\infty \qquad \text{i.e. } e^{-r/a}\to 1$$

(192) $$\boxed{\frac{d\sigma_k^{(1)}}{d\Omega} = \left[\frac{Ze^2}{4E_k\sin^2\frac{\vartheta}{2}}\right]^2}$$

$$E_k = \frac{\hbar^2k^2}{2m}$$

Rutherford scattering cross section of Coulomb potential