Integral Equation for Scattering Theory

The time-independent Schrödinger equation for a particle scattered from a fixed potential is

$$(H_0 + V)|\psi\rangle = E|\psi\rangle \quad \cdots\cdots (1)$$

where H_0 is the kinetic energy operator. In the coordinate representation Eq. (1) can be written as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

or,

$$(\nabla^2 + k^2)\psi(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r})\psi(\vec{r}) \quad \cdots\cdots (2)$$

where

$$k^2 = \frac{2mE}{\hbar^2}.$$

We have to solve the time-independent Schrödinger equation subject to the boundary condition

$$\psi(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r}. \quad \cdots\cdots (3)$$

We can convert the Schrödinger equation into an integral equation in which the boundary condition (3) is incorporated. First, we define the Green's function $G(\vec{r}, \vec{r}')$ as follows;

$$\left(\nabla^2 + k^2\right) G(\vec{r}, \vec{r}') = \frac{2m}{\hbar^2} \delta(\vec{r} - \vec{r}') \quad \cdots \quad (4)$$

The Green's function can be interpreted as the effect or response at the point $\vec{r}$ due to a unit source at the point $\vec{r}'$. Now, if the Green's function is known, then the function $\psi(\vec{r})$ which is given by the integral relation

$$\psi(\vec{r}) = \int G(\vec{r}, \vec{r}')\, V(\vec{r}')\, \psi(\vec{r}') \quad \cdots \quad (5)$$

satisfies Eq. (2). Indeed, operating by $(\nabla^2 + k^2)$ on this equation we get

$$(\nabla^2 + k^2)\psi(\vec{r})$$

$$= (\nabla^2 + k^2)\int G(\vec{r},\vec{r}\,')V(\vec{r}\,')\psi(\vec{r}\,')d^3r'$$

$$= \int (\nabla^2 + k^2)G(\vec{r},\vec{r}\,')V(\vec{r}\,')\psi(\vec{r}\,')d^3r'$$

$$= \frac{2m}{\hbar^2}\int \delta(\vec{r}-\vec{r}\,')V(\vec{r}\,')\psi(\vec{r}\,')d^3r'$$

$$= \frac{2m}{\hbar^2}V(\vec{r})\psi(\vec{r})$$

which is just the Schrödinger equation. Now, in order to get the complete solution of Eq. (2) we should add to Eq. (5) a function $\phi(\vec{r})$ which is a solution of the homogeneous equation

$$(\nabla^2 + k^2)\phi(\vec{r}) = 0 \quad \cdots\cdots\cdots (6)$$

We take $\phi(\vec{r}) = e^{ikz}$ which corresponds to a plane wave propagating along the positive z-axis.

Then the most general solution which satisfies Eq. (2) can be written in the form

$$\psi(\vec{r}) = \phi(\vec{r}) + \int G(\vec{r}, \vec{r}\,')V(\vec{r}\,')\,\psi(\vec{r}\,')\,d^3r' \quad \cdots (7)$$

Note that the presence of $\psi(\vec{r}\,')$ on the right hand side of this equation makes it an integral equation. The Green's function must be such that the outgoing boundary condition for $\psi(\vec{r})$, Eq. (3), is satisfied. The integral equation (7) is called the Lippmann Schwinger equation.

Calculation of the Green's function

We now have to find the Green's function defined by Eq. (4). First, we note that the Fourier decomposition of $\delta(\vec{r}-\vec{r}\,')$ is

$$\delta(\vec{r}-\vec{r}\,') = \frac{1}{(2\pi)^3}\int e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}\, d^3k' . \quad \cdots\ (8)$$

Next, let us write the Fourier decomposition of $G(\vec{r},\vec{r}\,')$ as

$$G(\vec{r},\vec{r}\,') = \frac{1}{(2\pi)^3}\int g(k')\, e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}\, d^3k' \quad \cdots\ (9)$$

where we have to find the function $g(k')$. To do so we substitute Eq. (8) and (9) in Eq. (4). We get

$$\frac{1}{(2\pi)^3}\int (-k'^2+k^2)\, g(k')\, e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}\, d^3k'$$

$$= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}\, d^3k'$$

From this we see that

$$(-k'^2 + k^2)\, g(k') = \frac{2m}{\hbar^2}.$$

Except for $k' = k$, the function $g(k')$ is then

$$g(k') = \frac{2m}{\hbar^2} \; \frac{1}{k^2 - k'^2}. \quad \cdots\cdots (10)$$

Using this value of $g(k')$ in Eq. (9) we find

$$G(\vec{r}, \vec{r}\,') = \frac{2m}{\hbar^2} \cdot \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}' \cdot (\vec{r} - \vec{r}\,')}}{k^2 - k'^2}\, d^3k' \cdots (11)$$

We can directly do the angular integrals in Eq (11) as follows. First, define a vector $\vec{R}$ as

$$\vec{R} = \vec{r} - \vec{r}\,'$$

which is fixed as we integrate over k'. Let the z-axis of the coordinate system be aligned in the direction of $\vec{R}$, and suppose that θ is the angle between $\vec{k}'$ and $\vec{R}$. So, θ is the polar angle of the vector $\vec{k}'$.

Eq. (11) is now written as

$$G(\vec{r},\vec{r}\,') = \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int \frac{e^{ik'R\cos\theta}\, k'^2 dk' \sin\theta\, d\theta\, d\phi}{(k^2-k'^2)}$$

$$= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^\infty \frac{k'^2 dk'}{(k^2-k'^2)}\int_0^\pi e^{ik'R\cos\theta}\sin\theta\, d\theta \int_0^{2\pi} d\phi$$

$$= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\cdot 2\pi \int_0^\infty \frac{k'^2 dk'}{(k^2-k'^2)}\int_{-1}^{+1} e^{ik'R\mu}\, d\mu$$

where we have made a change of variable:

$$\mu = \cos\theta .$$

The μ-integral is easy to perform:

$$\int_{-1}^{+1} e^{ik'R\mu}\, d\mu = \frac{1}{ik'R}\left(e^{ik'R} - e^{-ik'R}\right)$$

Hence

$$G(\vec{r},\vec{r}\,') = \frac{2m}{\hbar^2}\frac{1}{4\pi^2 iR}\int_0^\infty \frac{k'(e^{ik'R}-e^{-ik'R})}{(k^2-k'^2)}dk'$$

The integrand is an even function of k'.
Therefore we have

$$G(\vec{r},\vec{r}') = \frac{2m}{\hbar^2}\frac{1}{4\pi^2 i R}\frac{1}{2}\int_{-\infty}^{\infty}\frac{k'(e^{ik'R}-e^{-ik'R})}{(k^2-k'^2)}dk'$$

$$= \left(\frac{2m}{\hbar^2}\right)\frac{1}{8\pi^2 i R}(I_1 - I_2) \quad \text{------}(12)$$

where we have defined

$$I_1 = \int_{-\infty}^{\infty}\frac{k' e^{ik'R}}{(k^2-k'^2)}dk' \quad \text{------}(13)$$

and

$$I_2 = \int_{-\infty}^{\infty}\frac{k' e^{-ik'R}}{(k^2-k'^2)}dk'. \quad \text{------}(14)$$

The integrals I_1 and I_2 are not defined because the integrands have singularities at $k'=k$ and $k'=-k$. Unless we specify how to avoid these singularities, Green's function cannot be calculated.

In order to overcome the difficulty, we think of k' as a complex variable and do the integrals I_1 and I_2 in the complex k'-plane over contours which include the real k'-axis and deforming the contours such that we get the Green's function which leads to outgoing spherical waves. The procedure is explained below.

Calculation of I_1

First, let us consider the integral I_1, Eq. (13). The exponential term $e^{ik'R}$ in the integral can be written as

$$e^{ik'R} = e^{i(\mathrm{Re}\, k')R}\, e^{-(\mathrm{Im}\, k')R}.$$

This suggests that we close the contour in the upper half plane, $\mathrm{Im}\, k' > 0$, by a large semicircle so that the contribution to this integral from the semi circle tends to zero as we let the radius tend to infinity.

In Fig. 1 below we show the contour for doing the integral I_1 so that we get outgoing waves.

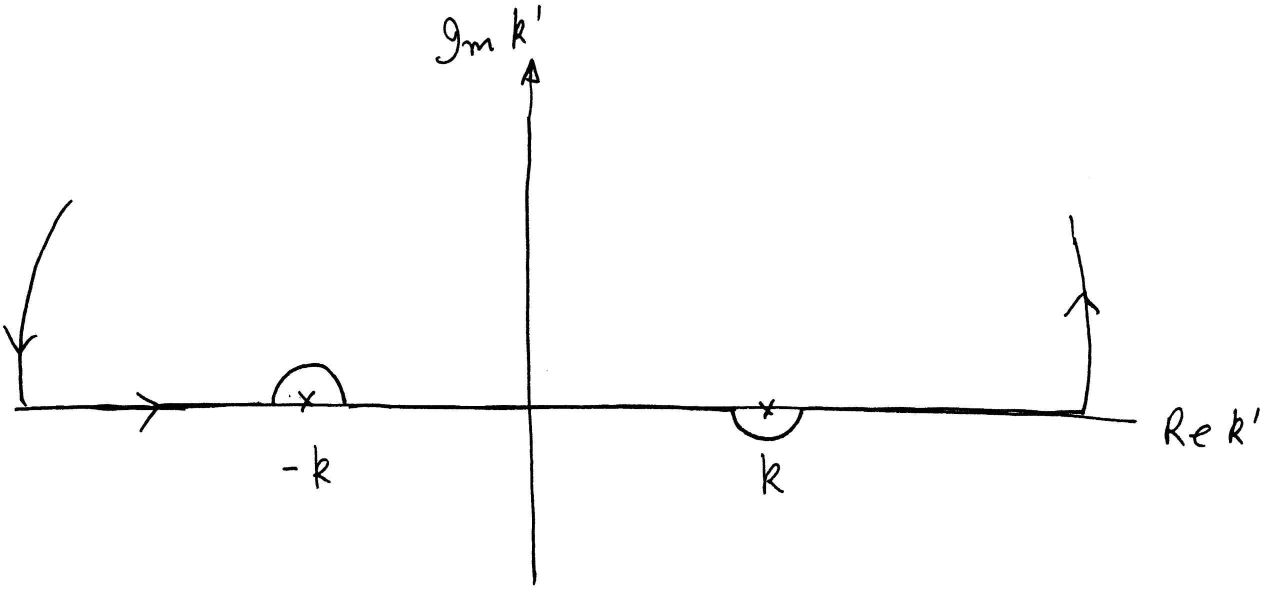

Fig 1. Contour for the integral I_1, Eq. (13).

We have deformed the contour around the singularities $k' = -k$ and $k' = k$ in such a manner so as to include the singularity at k within the contour and exclude the singularity at $-k$. Then,

$$\oint_c \frac{k' e^{ik'R}}{(k^2 - k'^2)} dk' = 2\pi i \sum \text{Res} .$$

Since the infinite semicircle contributes nothing to the integral

$$I_1 = \int_{-\infty}^{\infty} \frac{k' e^{ik'R}}{(k^2 - k'^2)} dk' = 2\pi i \, \mathrm{Res}\left(\frac{k' e^{ik'R}}{(k^2 - k'^2)} \right)_{k'=k}$$

or,

$$I_1 = 2\pi i \lim_{k' \to k} (k' - k) \frac{k' e^{ik'R}}{(k - k')(k + k')}$$

$$= 2\pi i (-1) \frac{\cancel{k} e^{ikR}}{2 \cancel{k}}$$

$$= -\pi i e^{ikR} \qquad \cdots\cdots (15).$$

If we had deformed the contour in Fig. 1 to include the singularity at $-k$ and exclude the one at k from the interior of the contour, we would get $I_1 \propto e^{-ikR}$ which leads to the incoming boundary condition for the wave function.

Calculation of I_2

The integral I_2 is given in Eq. (14). Since the exponential function in the integrand of I_2 is

$$e^{-ik'R} = e^{-i(\mathrm{Re}\,k')r}\, e^{(\mathrm{Im}\,k')R},$$

we need to close the contour by an infinite semi circle in lower half of the k'-plane. We deform the contour (Fig. 2) on the real k'-axis to include the singularity at $-k$ and exclude the singularity at k from the region inside the contour.

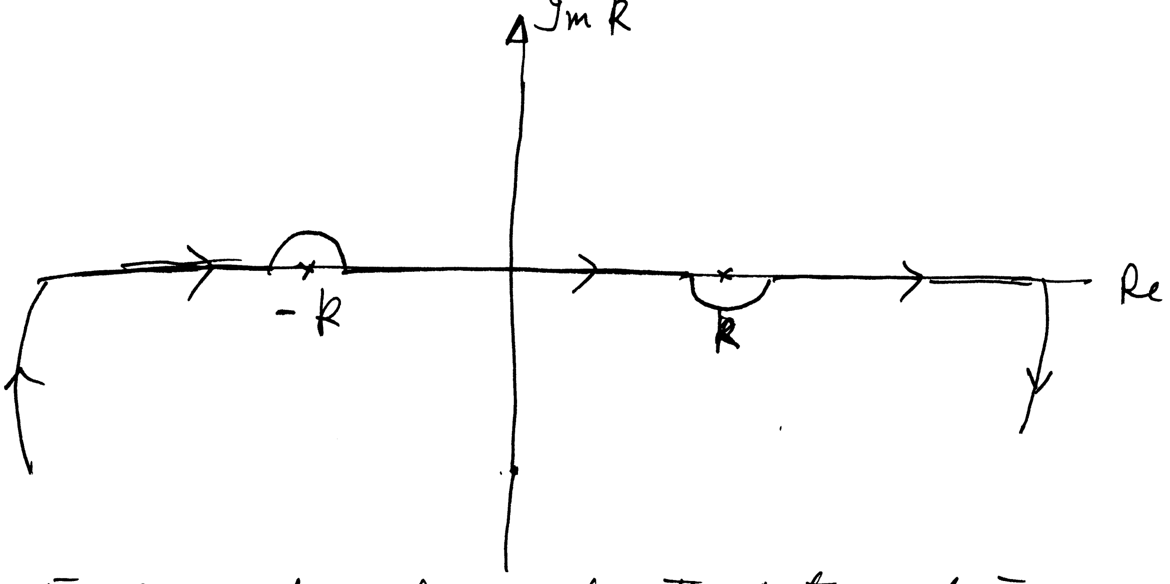

Fig. 2 Contour chosen for the integral I_2.

Then

$$I_2 = \int_{-\infty}^{\infty} \frac{k' e^{-ik'R}}{(k^2 - k'^2)}$$

$$= -2\pi i \; \mathrm{Res}\left(\frac{k' e^{-ik'R}}{(k-k')(k+k')} \right)_{k' = -k}$$

$$= -2\pi i \lim_{k' \to -k} \cancel{(k'+k)} \frac{k' e^{-ik'R}}{(k-k')\cancel{(k+k')}}$$

$$= -2\pi i \; \frac{-k e^{ikR}}{2k}$$

$$= \pi i e^{ikR} \quad \text{- - - - - - - - - - (16)}$$

which also leads to an outgoing wave.

Final expression for $G(\vec{r}, \vec{r}\,')$.

We now substitute (15) and (16) in (11).
We get

$$G(\vec{r}, \vec{r}\,') = \frac{2m}{\hbar^2} \frac{1}{8\pi^2 i R} \left(-\pi i e^{ikR} - \pi i e^{ikR} \right)$$

$$= -\frac{2m}{\hbar^2} \frac{1}{8\pi^2 i R} 2\pi i e^{ikR}$$

$$= -\frac{2m}{\hbar^2} \frac{1}{4\pi R} e^{ikR}$$

i.e.,

$$G^{(+)}(\vec{r}, \vec{r}\,') = -\frac{2m}{\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{4\pi |\vec{r}-\vec{r}\,'|} . \quad \cdots \text{(17)}$$

This Green's function has outgoing boundary condition. We have put a superscript "(+)" in G to signify the outgoing ~~scattered~~ boundary condition.

The $\pm i\epsilon$ prescription

We note that we could have obtained the same result for $G^{(+)}(\vec{r},\vec{r}\,')$ by pushing up the pole at $k' = k$ slightly above the real axis and the pole at $k' = -k$ slightly below the axis and using the contours as shown in figure (3).

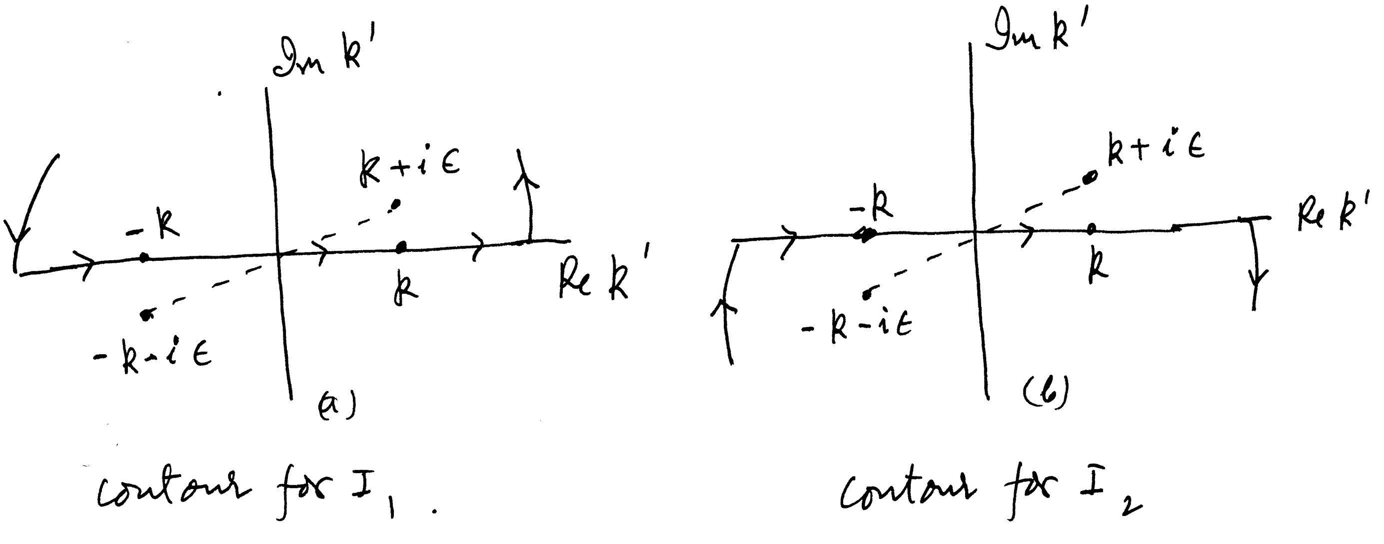

Fig 3. Contours for the integrals I_1 (a) and for I_2 (b). The part of the contours along the real k' axis is undeformed. Instead the poles $\pm k$ are shifted to $\pm ik \pm i\epsilon$.

This could be achieved by replacing k by $k+i\epsilon$ where ϵ is a positive infinitesimal quantity $\epsilon \to 0^+$. Then

$$(k^2 - k'^2) = (k-k')(k+k') \longrightarrow (k+i\epsilon-k')(k+i\epsilon+k')$$

so that the poles are now at $k' = k+i\epsilon$ and $k' = -k - i\epsilon$. Replacing k by $k+i\epsilon$, where ϵ is an infinitesimal, amounts to

$$k^2 \to (k+i\epsilon)^2 = k^2 + 2ki\epsilon - \epsilon^2$$

$$= k^2 + i\epsilon \qquad \Big| \; 2k\epsilon \text{ is also an infinitesimal}$$

so that

$$k^2 - k'^2 \longrightarrow k^2 - k'^2 + i\epsilon .$$

Therefore, using this prescription in Eq. (11) we get

$$G^{(+)}(\vec{r}, \vec{r}\,') = \frac{2m}{\hbar^2} \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}' \cdot (\vec{r} - \vec{r}\,')}}{k^2 - k'^2 + i\epsilon} \, d^3k'$$

Doing this integral would lead to the outgoing Green's function given in Eq. (17).

If instead we push the pole at $k' = k$ to the lower half plane and the pole at $k' = -k$ to the upper half plane by substituting $k^2 \rightarrow k^2 - i\epsilon$, as shown in Fig. (4), we will get the Green's function with incoming boundary condition:

$$G^{(-)}(\vec{r}, \vec{r}\,') = -\frac{2m}{\hbar^2} \cdot \frac{e^{-ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|} \quad \text{--- (18)}$$

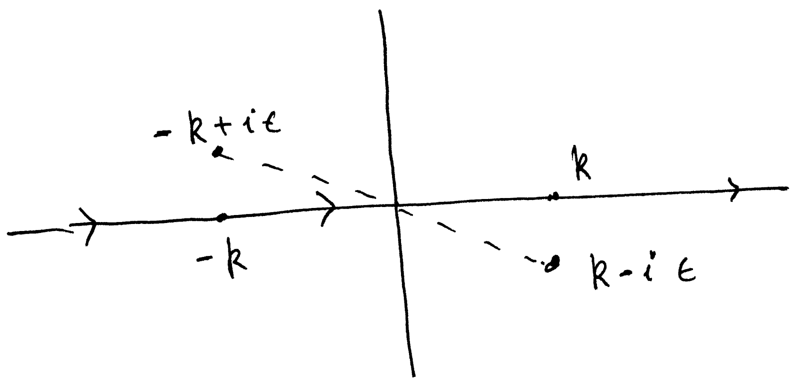

Fig. 4 The shift of the poles at $k' = \pm k$ for the incoming Green's function. The contour is closed in the upper half plane for the integral I_1 and in the lower half plane for the integral I_2.

Integral equation for $\psi(\vec{r})$

The full wave function $\psi^{(+)}(\vec{r})$ with the outgoing boundary condition (Eq. (3)) can now be written down:

$$\psi^{(+)}(\vec{r}) = \phi(\vec{r}) + \int G^{(+)}(\vec{r},\vec{r}\,')\, V(\vec{r}\,')\, \psi(\vec{r}\,')\, d^3r'$$

$$= \phi(\vec{r}) + \frac{2m}{\hbar^2}\left(-\frac{1}{4\pi}\right)\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\, V(\vec{r}\,')\, \psi^{(+)}(\vec{r}\,')\, d^3r'$$

i.e.,

$$\psi^{(+)}(\vec{r}) = \phi(\vec{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\, V(\vec{r}\,')\, \psi^{(+)}(\vec{r}\,')\, d^3r'. \quad \ldots\ldots(19)$$

We have take $\phi(\vec{r})$ to represent a plane wave propagating along the z-axis, i.e.,

$$\phi(\vec{r}) = e^{ikz}.$$

Equation (19) is called the Lippmann-Schwinger equation for the wave function with outgoing boundary condition.

Using the Green's function $G^{(-)}(\vec{r}, \vec{r}\,')$ would give us the wavefunction $\psi^{(-)}(\vec{r})$ with incoming boundary condition

$$\psi^{(-)}(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta,\varphi)\, e^{-ikr}/r \, .$$

The Scattering Amplitude.

The wave function $\psi^{(+)}(\vec{r})$ with outgoing boundary condition is (Eq. (19))

$$\psi^{(+)}(\vec{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} V(\vec{r}\,')\,\psi^{(+)}(\vec{r}\,')\, d^3r' \quad \text{--- (20)}$$

where we have taken e^{ikz} as the solution of the homogeneous equation $(V=0)$.

Suppose $V(\vec{r}\,')$ is localized about $\vec{r}=0$ (that is, the potential drops to zero outside some finite region, as is typical of scattering problem) and we want to calculate $\psi^{(+)}(\vec{r})$ at points far away from the scattering center. Then $|\vec{r}| >> |\vec{r}\,'|$ for all points that contribute to the integral in Eq. (20).

For large $|\vec{r}|$ (i.e., $r >> r'$) we can make the following approximation

$$|\vec{r} - \vec{r}'| = (r^2 - 2\vec{r}\cdot\vec{r}' + r'^2)^{1/2}$$

$$\simeq r\left(1 - \frac{\vec{r}\cdot\vec{r}'}{r}\right)$$

$$= r - \frac{\vec{r}\cdot\vec{r}'}{r}$$

$$= r - \hat{r}\cdot\vec{r}'$$

Also

$$\frac{1}{|\vec{r} - \vec{r}'|} \simeq \frac{1}{r\left(1 - \frac{\hat{r}\cdot\vec{r}'}{r}\right)}$$

$$= \frac{1}{r}\left(1 - \frac{\hat{r}\cdot\vec{r}'}{r}\right)^{-1}$$

$$\simeq \frac{1}{r}\left(1 + \frac{\hat{r}\cdot\vec{r}'}{r}\right)$$

$$= \frac{1}{r} + O\left(\frac{1}{r^2}\right)$$

Therefore,

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \underset{r\to\infty}{\sim} \frac{e^{ik(r-\hat{r}\cdot\vec{r}')}}{r}$$

$$= \frac{e^{ikr}}{r} e^{-ik\hat{r}\cdot\vec{r}'}$$

$$= \frac{e^{ikr}}{r} e^{-i\vec{k}'\cdot\vec{r}'}$$

where we have defined

$$\vec{k}' = k\hat{r},$$

i.e., $\vec{k}'$ represents a wave vector of magnitude k in the outgoing direction $\hat{r}$. Defining the wave vector $\vec{k}$ of the same magnitude k in the incident direction, i.e., $\vec{k} = k\hat{z}$, the asymptotic form of Eq. (20) is

$$\psi^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\cdot\frac{e^{ikr}}{r}\int e^{-i\vec{k}'\cdot\vec{r}'} V(\vec{r}')\psi^{(+)}(\vec{r}')d^3r'.$$

This is in the standard form (Eq. 3) and we can read off ~~the~~ the scattering amplitude:

$$f(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int e^{-i\vec{k}'\cdot\vec{r}'} V(\vec{r}')\,\psi^{(+)}(\vec{r}')\,d^3r' \quad \cdots\cdots (21)$$

where $\psi^{(+)}(\vec{r}')$ is given by Eq. (20). This is the exact integral expression for the scattering amplitude.

<u>Born approximation for the scattering amplitude.</u>

Suppose the incoming wave is not substantially altered by the potential, either because the potential is weak or ~~the par~~ because the particle has high energy. Then it makes sense to use

$$\psi^{(+)}(\vec{r}') \simeq \phi(\vec{r}') = e^{i\vec{k}\cdot\vec{r}'}$$

inside the integral of Eq. (21). This approximation is called the Born approximation. In the Born approximation, Then

$$f_B(\theta,\varphi) \cong -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'}\, V(\vec{r}')\, d^3r' \qquad (22)$$

Defining

$$\vec{q} = \vec{k} - \vec{k}'$$

we write

$$f_B(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int e^{i\vec{q}\cdot\vec{r}'}\, V(\vec{r}')\, d^3r' \quad \cdots\cdots (23)$$

The vector $\hbar\vec{q}$ is called the momentum transfer in the scattering process. From Eq. (23) we see that, apart from a multiplicative factor, f_B is the Fourier transform of the potential. The two wave vectors $\vec{k}$ and $\vec{k}'$ and $\vec{q}$ are shown in the figure below:

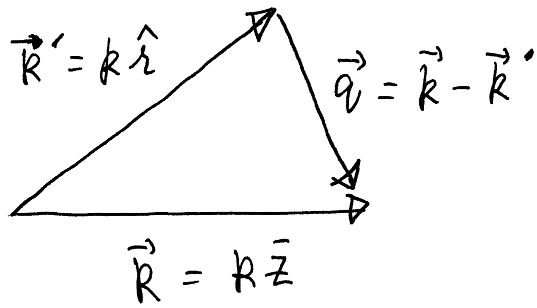

Fig. The wave vectors in the Born approximation: $\vec{k}$ points in the incident direction and $\vec{k}'$ points in the scattered direction.

From the figure we see that

$$q^2 = |\vec{k}|^2 + |\vec{k}'|^2 - 2|\vec{k}||\vec{k}'|\cos\theta$$

$$= k^2 + k^2 - 2k^2\cos\theta$$

$$= 2k^2(1-\cos\theta)$$

$$= 4k^2\sin^2\theta/2$$

i.e.,

$$q = 2k\sin\theta/2$$

For low-energy particles (long wavelength), we can make a further approximation. In the case of low-energy scattering, the exponential factor in f_B (Eq. (22)) is essentially constant over the integration region, and the Born approximation formula for f_B simplifies to

$$f_B(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int V(\vec{r})\,d^3r . \qquad (24)$$

(low-energy)

<u>Central potential</u>

If the potential is central, i.e., $V = V(|\vec{r}|) = V(r)$, the scattering amplitude would be a function of θ only. For a central potential, it is easy to do the angular integrals in Eq. (23) quite easily since V has no angular dependence.

First, write Eq. (23) in the form

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{iqr'\cos\theta}\, V(r')\, r'^2 dr' \sin\theta\, d\theta\, d\varphi$$

where θ is the angle between $\vec{q}$ and $\vec{r}\,'$ and φ is the azimuthal angle of $\vec{r}\,'$ around $\vec{q}$ measured from a certain reference direction perpendicular to $\vec{q}$.

Since θ varies from 0 to π, and φ can vary from 0 to 2π, we have

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2}\int_0^\infty dr'\, r'^2 V(r')\int_0^\pi e^{iqr'\cos\theta}\sin\theta\, d\theta\int_0^{2\pi} d\varphi$$

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

where we have made a change of variable

$$\mu = \cos\theta$$

Now

$$\int_{-\infty}^{\infty} e^{iqr'\mu}\, d\mu = \frac{1}{iqr'}\, e^{iqr'\mu}\Big|_{\mu=-1}^{\mu=1}$$

$$= \frac{1}{iqr'}\left(e^{iqr'} - e^{-iqr'}\right)$$

$$= \frac{2\sin qr'}{qr'}$$

Therefore,

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

or

$$f_B(\theta) = \frac{2m}{\hbar^2 q}\int_0^{\infty} dr'\, r'\, V(r') \sin qr'. \qquad \ldots (27)$$

The θ-dependence of $f_B(\theta)$ comes from q which is

$$q = 2k\sin\theta/2$$

Examples of application of Born approximation

Ex Low-energy soft-sphere scattering

Suppose

$$V(r) = \begin{cases} V_0 & \text{if } r \lesssim a \\ 0 & \text{if } r > a. \end{cases}$$

In case of low-energy scattering we can use Eq. (24), i.e.,

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2}\int V(\vec{r})\, d^3r$$

Since $V(r)$ is constant,

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2} \cdot V_0 \left(\frac{4}{3}\pi a^3\right)$$

$$= \frac{2mV_0 a^3}{3\hbar^2},$$

which is actually independent of θ and φ. The differential cross-section is

$$\frac{d\sigma}{d\Omega} = |f|^2 = \left(\frac{2mV_0 a^3}{3\hbar^2}\right)^2$$

and the total cross-section is

$$\sigma = 4\pi \left(\frac{2 m V_0 a^3}{3 \hbar^2} \right)^2 .$$

<u>Ex</u> Square-well potential

$$V(r) = \begin{cases} -V_0 & \text{for } r \le a \\ 0 & \text{for } r > a \end{cases}$$

In the Born approximation, the scattering amplitude is

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

where $q = |\vec{k} - \vec{k}'| = 2k \sin \theta/2$.

For the square-well potential, $f_B(\theta)$ is

$$f_B(\theta) = \frac{2 m V_0}{\hbar^2 q} \int_0^a r \sin qr \, dr$$

$$= \frac{2 m V_0}{\hbar^2 q^3} \int_0^{qa} qr \sin qr \, d(qr)$$

or

$$f_B(\theta) = \frac{2mV_0}{\hbar^2 q^3} \int_0^{qa} \xi \sin\xi \, d\xi$$

where $\xi = qr$.

Now,

$$\int_0^{qa} \xi \sin\xi \, d\xi = -\int_0^{qa} \xi \, d(\cos\xi)$$

$$= -\left[\xi\cos\xi \Big|_0^{qa} - \int_0^{qa} \cos\xi \, d\xi \right]$$

$d(fg) = f\,dg + g\,df$

$\therefore \int f\,dg = fg - \int g\,df$

$$= -\left[\xi\cos\xi \Big|_0^{qa} - \sin\xi \Big|_0^{qa} \right]$$

$$= \sin qa - qa\cos qa$$

Therefore,

$$f_B(\theta) = \frac{2mV_0}{\hbar^2 q^3} (\sin qa - qa\cos qa)$$

or

$$f_B(\theta) = \frac{2mV_0 a^3}{\hbar^2} \left[\frac{\sin qa - qa\cos qa}{(qa)^3} \right]$$

The differential cross-section is then

$$\frac{d\sigma}{d\Omega}(\theta) = |f_B(\theta)|^2$$

$$= \left(\frac{2mV_0a^3}{\hbar^2}\right)^2 \left[\frac{\sin qa - qa\cos qa}{(qa)^3}\right]^2$$

Let $\eta = qa$. Therefore

$$\frac{d\sigma}{d\Omega}(\theta) = \left(\frac{2mV_0a^3}{\hbar^2}\right)^2 \left(\frac{\sin\eta - \eta\cos\eta}{\eta^3}\right)^2$$

or,

$$\frac{d\sigma}{d\Omega}(\theta) = \left(\frac{2mV_0a^3}{\hbar^2}\right)^2 g(\eta).$$

The θ-dependence of the differential cross section comes from the function $g(\eta)$ where

$$\eta = qa = 2k\sin\frac{\theta}{2}\cdot a = 2ka\sin\theta/2.$$

Low-energy limit of the differential cross-section.

For low energy $\eta = qa \ll 1$. In the limit of small η we have

$$\frac{\sin\eta - \eta\cos\eta}{\eta^3}$$

$$= \frac{(\eta - \eta^3/3! + \eta^5/5! - \cdots) - \eta(1 - \eta^2/2! + \eta^4/4! - \cdots)}{\eta^3}$$

$$= \frac{-\eta^3/6 + \eta^5/5! \cdots + \eta^3/2 - \eta^5/4! + \cdots}{\eta^3}$$

$$= \frac{\eta^3/3 - \eta^5/30 + \cdots}{\eta^3}$$

$$= \frac{1}{3} - \eta^2/30 + \cdots$$

$$\therefore \quad g(\eta) = \left(\frac{\sin\eta - \eta\cos\eta}{\eta^3} \right)^2$$

$$\simeq \frac{1}{9} + O(\eta^2)$$

Therefore,

$$\frac{d\sigma}{d\Omega}(\theta) = \left(\frac{2mV_0 a^3}{\hbar^2} \right)^2 \frac{1}{9}$$

or $$\frac{d\sigma}{d\Omega}(\theta) = \left(\frac{2mV_0 a^3}{3\hbar^2} \right)^2 \text{(independent of } \theta\text{)}.$$

We could find the low-energy limit of the differential cross-section by proceeding as in the first example of low-energy scattering from a soft sphere.

Ex Screened Coulomb potential

Screened coulomb potential is of the form

$$V(r) = \frac{Ze^2}{4\pi\epsilon_0 r} e^{-r/a}$$

Since the potential is central, the scattering amplitude in the Born approximation can be written as

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

where

$$q = |\vec{k} - \vec{k}'| = 2k \sin \theta/2$$

For the screened coulomb potential we have

$$f_B(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty dr\, \cancel{r}\, \frac{Ze^2}{4\pi\epsilon_0 \cancel{r}} e^{-r/a} \sin q r$$

$$= -\frac{2m}{\hbar^2 q}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\int_0^\infty e^{-r/a} \sin q r\, dr$$

$$= -\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\frac{2m}{\hbar^2 \cancel{q}} \cdot \frac{\cancel{q}}{q^2 + \frac{1}{a^2}} \quad \text{(see note below)}$$

$$= -\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\frac{2m}{\hbar^2} \cdot \frac{a^2}{q^2 a^2 + 1}$$

Point Coulomb interaction

For point coulomb interaction we have

$$V(r) = \frac{Ze^2}{4\pi\epsilon_0 r}$$

The scattering amplitude for point Coulomb interaction in the Born approximation is

$$f_B(\theta) = -\frac{2m}{\hbar^2 q}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)\int_0^\infty \sin qr\, dr$$

The integral is undefined because $\sin qr$ is oscillatory as $r \to \infty$. One way to get around the difficulty is to include a convergence factor $e^{-r/a}$ in the integrand and let $a \to \infty$ at the end. Therefore $f_B(\theta)$ for point Coulomb interaction can be obtained by taking the limit $a \to \infty$ of the amplitude for Screened Coulomb interaction. Thus

$$f_B^{\text{point Coul}}(\theta) = -\frac{Ze^2}{4\pi\epsilon_0}\cdot\frac{2m}{\hbar^2}\cdot\frac{a^2}{q^2 a^2}$$

$$= -\frac{Ze^2}{4\pi\epsilon_0}\;\frac{2m}{\hbar^2 q^2}$$

Now

$$q = 2k \sin\theta/2$$

or

$$q^2 = 4k^2 \sin^2\theta/2$$

$$= 4\,\frac{2mE}{\hbar^2}\sin^2\theta/2$$

$$= \frac{8mE}{\hbar^2}\sin^2\theta/2$$

Therefore

$$f_B(\theta) = -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{2m}{\cancel{\hbar^2}}\cdot\frac{\cancel{\hbar^2}}{8mE\sin^2\theta/2}$$

$$= -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{1}{4E\sin^2\theta/2}$$

$$= -\frac{Ze^2}{4\pi\epsilon_0\hbar c}(\hbar c)\,\frac{1}{4E\sin^2\theta/2}$$

$$= -Z\alpha\,(\hbar c)\,\frac{1}{4E\sin^2\theta/2}$$

$\alpha = \dfrac{e^2}{4\pi\epsilon_0\hbar c} = \dfrac{1}{137}$

Fine structure constant

$$= -\frac{Z\alpha(\hbar c)}{4E\sin^2\theta/2}$$

$$\therefore \quad \frac{d\sigma}{d\Omega}(\theta) = |f_B(\theta)|^2 = \frac{Z^2\alpha^2(\hbar c)^2}{16E^2\sin^4\theta/2}$$

This is the Rutherford formula.

Note:

We want to integrals like

$$\int_0^\infty e^{-\alpha r}\sin\beta r \, dr$$

or

$$\int_0^\infty e^{-\alpha r}\cos\beta r \, dr .$$

These integrals can be done by integration in parts twice. However, there is a simpler method illustrated below:

consider the integral

$$\int_0^\infty e^{-\alpha r} e^{i\beta r} dr = \int_0^\infty e^{-(\alpha - i\beta) r} dr$$

$$= -\frac{1}{(\alpha - i\beta)} e^{-(\alpha - i\beta)r}\Big|_0^\infty = \frac{1}{\alpha - i\beta} = \frac{\alpha}{(\alpha^2+\beta^2)} + \frac{i\beta}{(\alpha^2+\beta^2)}$$

Equating real and imaginary parts on both sides of the above equation

$$\int_0^\infty e^{-\alpha r} \cos\beta r \, dr = \frac{\alpha}{\alpha^2+\beta^2}$$

$$\int_0^\infty e^{-\alpha r} \sin\beta r \, dr = \frac{\beta}{\alpha^2+\beta^2}$$

<u>Ex</u> Yukawa potential

$$V(r) = \beta \, \frac{e^{-\mu r}}{r}$$

Similar to ~~point~~ screened Coulomb interaction, $V(r) = \dfrac{Ze^2}{4\pi\epsilon_0 r} e^{-r/a}$

$$\beta \longleftrightarrow \frac{Ze^2}{4\pi\epsilon_0}$$

$$\mu \longleftrightarrow \frac{1}{a}$$

Validity of Born approximation

Born approximation is based on the assumption that the potential causes very little change to the incoming free wave function e^{ikz}, i.e.,

$$\psi(\vec{r}) \simeq e^{ikz}$$

Since

$$\psi(\vec{r}) = e^{ikz} + \psi_{sc}(\vec{r})$$

we have

$$|\psi_{sc}(\vec{r})| << |e^{ikz}|$$

i.e.,

$$|\psi_{sc}(\vec{r})| << 1 \quad \text{for all } \vec{r}.$$

Now, the Lippman Schwinger equation for $\psi(\vec{r})$ is

$$\psi^{(+)}(\vec{r}) = e^{ikz} + \int G^{(+)}(\vec{r},\vec{r}\,')\,V(\vec{r}\,')\,\psi^{(+)}(\vec{r}\,')\,d^3r'$$

$$= e^{i\vec{k}\cdot\vec{r}} + \underbrace{\int G^{(+)}(\vec{r},\vec{r}\,')\,V(\vec{r}\,')\,\psi^{(+)}(\vec{r}\,')\,d^3r'}_{\psi_{sc}(\vec{r})}$$

The wave function in the Born approximation is obtained by replacing $\psi(\vec{r}')$ on the right hand side of the above equation by the plane wave $e^{i\vec{k}\cdot\vec{r}'}$.

Thus

$$\psi_B(\vec{r}) = \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{incoming plane wave}} + \underbrace{\int G^{(+)}(\vec{r},\vec{r}')\, V(\vec{r}')\, e^{i\vec{k}\cdot\vec{r}'}\, d^3r'}_{\text{Scattered wave } \psi_{sc}(\vec{r})}$$

$\psi_{sc}(\vec{r})$ is a small correction to $e^{i\vec{k}\cdot\vec{r}}$.

Hence condition for validity of Born approximation is

$$\left| \int G^{(+)}(\vec{r},\vec{r}')\, V(\vec{r}')\, e^{i\vec{k}\cdot\vec{r}'}\, d^3r' \right| << \left| e^{i\vec{k}\cdot\vec{r}} \right| = 1$$

Now, $$G^{(+)}(\vec{r},\vec{r}') = -\frac{2m}{\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|}$$

Therefore,

$$\frac{2m}{\hbar^2} \frac{1}{4\pi} \left| \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}')\, e^{i\vec{k}\cdot\vec{r}'}\, d^3r' \right| << 1$$

Since the scattered wave is the strongest at the origin, it is sufficient to satisfy the condition at $\vec{r} = 0$. Therefore,

$$\frac{2m}{\hbar^2} \frac{1}{4\pi} \left| \int \frac{e^{ikr'}}{r'} V(\vec{r}') e^{i\vec{k}\cdot\vec{r}'} r'^2 dr' \sin\theta \, d\theta \, d\varphi \right| << 1$$

If the potential is spherically symmetric, there is no angular dependence from the potential and the angular integration in the above equation becomes very simple. The angular integral is

$$\int e^{i\vec{k}\cdot\vec{r}'} \sin\theta \, d\theta \, d\phi$$

$$= \int_0^{\pi} e^{ikr'\cos\theta} \sin\theta \, d\theta \int_0^{2\pi} d\varphi$$

$$= 2\pi \int_{-1}^{+1} e^{ikr'\mu} d\mu \qquad \Big| \; \mu = \cos\theta$$

$$= 2\pi \, \frac{e^{ikr'} - e^{-ikr'}}{ikr'} = 4\pi \frac{\sin kr'}{kr'} .$$

$$\therefore \quad \frac{2m}{\hbar^2} \left| \int_0^\infty dr'\, r'^2 \, \frac{e^{ikr'}}{r'} V(r') \, \frac{\sin kr'}{kr'} \right| << 1$$

or $$\frac{2m}{\hbar^2 k} \left| \int_0^\infty e^{ikr'} V(r') \sin kr' \, dr' \right| << 1$$

or $$\frac{m}{\hbar^2 k} \left| \int_0^\infty \left(e^{2ikr'} - 1\right) V(r') \, dr' \right| << 1$$

which can be satisfied for large k or when V is small. Thus, Born approximation is valid either at large energy or for weak potentials.

Operator form of Lippmann - Schwinger Equation.

Previously we introduced the Green's function $G(\vec{r}, \vec{r}\,')$ which satisfies the differential equation

$$(\nabla^2 + k^2)\, G(\vec{r}, \vec{r}\,') = \overset{2m/\hbar^2}{\downarrow}\delta(\vec{r} - \vec{r}\,') \quad \text{- - - - (1)}$$

Now, there are many different Green's function with different boundary conditions satisfying Eq. (1). We showed that the Green's function $G^{(+)}(\vec{r}, \vec{r}\,')$ and $G^{(-)}(\vec{r}, \vec{r}\,')$ satisfying the outgoing and incoming boundary condition, respectively, can be expressed as

$$G^{(\pm)}(\vec{r}, \vec{r}\,') = \frac{1}{(2\pi)^3}\left(\frac{2m}{\hbar^2}\right) \int \frac{e^{i\vec{k}\,'\cdot(\vec{r}-\vec{r}\,')}}{k^2 - k'^2 \pm i\epsilon}\, dk', \quad (2)$$

where ϵ is a positive infinitesimal which tends to zero.

Doing the integral we get

$$G^{(\pm)}(\vec{r},\vec{r}\,') = -\frac{2m}{\hbar^2}\,\frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|} \quad \cdots\cdots (3)$$

In terms of $G^{(\pm)}$, the integral equations for the wave functions $\psi^{(\pm)}$ are

$$\psi^{(\pm)}(\vec{r}) = \phi(\vec{r}) + \int G^{(\pm)}(\vec{r},\vec{r}\,')V(\vec{r}\,')\psi^{(\pm)}(\vec{r}\,')d^3r'. \quad \cdots (4)$$

This equation is called the Lippmann - Schwinger (LS) equation in the coordinate representation. Both $\psi^{(+)}$ and $\psi^{(-)}$ satisfy the Schrödinger equation, but $\psi^{(+)}$ has the outgoing boundary condition and $\psi^{(-)}$ has the incoming boundary condition, i.e.,

$$\psi^{(\pm)}(\vec{r}) \underset{r\to\infty}{\sim} e^{ikz} + f(\theta)\,\frac{e^{\pm ikr}}{r}. \qquad (5)$$

In scattering theory, we are interested in $\psi^{(+)}$.

Lippmann - Schwinger (LS) equation in operator form.

We can express the LS equation in a more general form independent of the basis. First, define the operators

$$G_k^{(\pm)} = \frac{1}{E - H_0 \pm i\epsilon} \quad \text{- - - - -} \quad (6)$$

where $E = \hbar^2 k^2/2m$ and H_0 is the kinetic energy operator. Then the matrix element $\langle \vec{r} | G_k^{(\pm)} | \vec{r}\,' \rangle$ of $G_k^{(\pm)}$ in the coordinate representation is nothing but the Green's function $G^{(\pm)}(\vec{r}, \vec{r}\,')$ defined previously. To verify this, consider

$$\langle \vec{r} | G_k^{(\pm)} | \vec{r}\,' \rangle = \langle \vec{r} | \frac{1}{E - H_0 \pm i\epsilon} | \vec{r}\,' \rangle$$

$$= \int d^3k' d^3k'' \langle \vec{r} | \vec{k}' \rangle \langle \vec{k}' | \frac{1}{E - H_0 \pm i\epsilon} | \vec{k}'' \rangle \langle \vec{k}'' | \vec{r}\,' \rangle$$

$$\text{- - -} (7)$$

where we have used the completeness condition of the momentum eigenstates $|\vec{k}\rangle$. These states are normalized as

$$\langle \vec{k} | \vec{k}' \rangle = \delta(\vec{k} - \vec{k}') \quad \cdots\cdots (8)$$

so that the completeness condition is

$$\int d^3k \, |\vec{k}\rangle\langle\vec{k}| = \hat{1} \, . \quad \cdots\cdots (9)$$

In the coordinate basis the momentum eigenstates are

$$\phi_{\vec{k}}(\vec{r}) \equiv \langle \vec{r} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \, . \quad \cdots\cdots (10)$$

The states $|\vec{k}\rangle$ are simultaneous eigenstates of the momentum operator $\hat{\vec{P}}$ and the free Hamiltonian operator $\hat{H}_0$:

$$\hat{\vec{P}} |\vec{k}\rangle = \hbar \vec{k} |\vec{k}\rangle \quad \cdots\cdots (11a)$$

$$H_0 |\vec{k}\rangle = \frac{\hbar^2 k^2}{2m} |\vec{k}\rangle \quad \cdots\cdots (11b)$$

We can now write Eq. (7) as

$$\langle \vec{r}\,|G_k^{(\pm)}|\,\vec{r}\,'\rangle$$

$$= \frac{1}{(2\pi)^3}\int d^3k'\,d^3k''\, e^{i\vec{k}'\cdot\vec{r}}\;\frac{\langle \vec{k}'|\vec{k}''\rangle}{E(k)-E(k')\pm i\epsilon}\; e^{-i\vec{k}''\cdot\vec{r}\,'}$$

$$= \frac{1}{(2\pi)^3}\int d^3k'\;\frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}}{\frac{\hbar^2k^2}{2m}-\frac{\hbar^2k'^2}{2m}\pm i\epsilon}$$

$$= \frac{2m}{\hbar^2}\cdot\frac{1}{(2\pi)^3}\int \frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}}{k^2-k'^2\pm i\epsilon}\,d^3k'$$

which is the Green's function found previously, Eq. (2).

The Lippmann-Schwinger equation can now written in a general form independent of basis. In coordinate representation, the Lippmann-Schwinger equation is given in Eq. (4). If we dispense with the coordinate basis, we can write simply

$$\boxed{|\psi_k^{(\pm)}\rangle = |\phi_k\rangle + G_k^{(\pm)} V |\psi_k^{(\pm)}\rangle} \quad \cdots (12)$$

To check whether this abstract equation gives us the Lippmann-Schwinger equation in the coordinate representation, we simply have to take the scalar product of this equation with $\langle\vec{r}|$:

$$\langle\vec{r}|\psi_k^{(\pm)}\rangle = \langle\vec{r}|\phi_k\rangle + \langle\vec{r}|G_k^{(\pm)} V |\psi_k^{(\pm)}\rangle$$

We now use the completeness of the basis set $|\vec{r}\rangle$ i.e.,

$$\int |\vec{r}\rangle\langle\vec{r}|\, d^3r = \hat{1}$$

to get

$$\langle\vec{r}|\psi_k^{(\pm)}\rangle = \langle\vec{r}|\phi_k\rangle + \int \langle\vec{r}|G_k^{(\pm)}|\vec{r}\,'\rangle\langle\vec{r}\,'|V|\vec{r}\,''\rangle\langle\vec{r}\,''|\psi_k^{(\pm)}\rangle \quad \cdots (13).$$

Now, suppose the potential operator is diagonal in coordinate space, i.e.,

$$\langle \vec{r}\,' | V | \vec{r}\,'' \rangle = V(\vec{r}\,')\,\delta(\vec{r}\,' - \vec{r}\,'') \quad \text{----(14)}$$

Such potentials are called local potentials. If V is not diagonal, then V would be called a non-local potential. All the potentials that we have worked with so far are local potentials. Non local potentials are hardly encountered in quantum mechanics.

Using Eq. (14) in Eq. (13) we have

$$\langle \vec{r} | \psi_k^{(\pm)} \rangle = \langle \vec{r} | \phi_k \rangle + \int \langle \vec{r} | G_k^{(\pm)} | \vec{r}\,' \rangle V(\vec{r}\,') \langle \vec{r}\,' | \psi_k^{(+)} \rangle$$

i.e.,

$$\psi_k^{(\pm)}(\vec{r}) = \phi_k(\vec{r}) + \int G^{(\pm)}(\vec{r}, \vec{r}\,') V(\vec{r}\,') \psi_k^{(\pm)}(\vec{r}\,')$$

which is the Lippmann - Schwinger Equation in coordinate space as was previously written down in Eq. (4).

Von Neumann series

The Lippmann-Schwinger equation in the operator form is given in Eq. (12), i.e.,

$$|\psi_k^{(\pm)}\rangle = |\phi_k\rangle + \frac{1}{E - H_0 \pm i\epsilon} V |\psi_k^{(\pm)}\rangle \qquad (15).$$

Iterating this equation, we get an infinite series:

$$|\psi_k^{(\pm)}\rangle = |\phi_k\rangle + \frac{1}{E - H_0 \pm i\epsilon} V |\phi_k\rangle + \frac{1}{E - H_0 \pm i\epsilon} V \frac{1}{E - H_0 \pm i\epsilon} V |\phi_k\rangle + \cdots \qquad (16)$$

This infinite series is called Von Neumann series. In coordinate representation, this series can be written as

$$\psi_k^{(\pm)}(\vec{r}) = \phi_k(\vec{r}) + \int G^{(\pm)}(\vec{r}, \vec{r}\,') V(\vec{r}\,') \phi_k(\vec{r}\,') d^3r' + \int G^{(\pm)}(\vec{r}, \vec{r}\,') V(\vec{r}\,') G^{(\pm)}(\vec{r}\,', \vec{r}\,'') V(\vec{r}\,'') \phi_k(\vec{r}\,'') d^3r' d^3r'' + \cdots \qquad (17).$$

Truncating the series at the second term is called the Born approximation. Thus in the Born approximation

$$|\psi_k^{(\pm)}\rangle_{Born} = |\phi_k\rangle + \frac{1}{E-H_0 \pm i\epsilon} V |\phi_k\rangle \quad ---(18)$$

i.e., in the coordinate representation

$$\psi_k^{(\pm)}(\vec{r}) = \phi_k(\vec{r}) + \int G^{(\pm)}(\vec{r},\vec{r}\,') V(\vec{r}\,') \phi_k(\vec{r}\,') d^3r' \quad ---(19)$$

Now, the first term in the Von Neumann series is called the unscattered term, the second term is called the single scattering term, the third term is called the double scattering term and so on. These terms can be diagramatically represented as shown in the figure below.

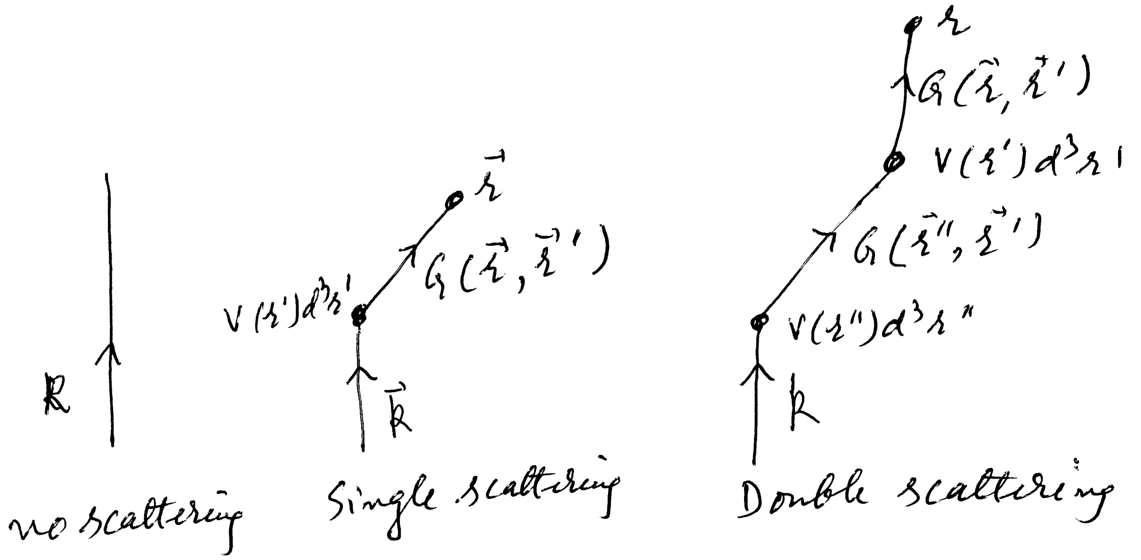

Fig. Diagramatic representation of Von Neumann series in coordinate space.

Formal solution of Lippmann - Schwinger Equation.

The Lippmann - Schwinger (LS) equation in operator form is

$$|\psi_k^{(\pm)}\rangle = |\phi_k\rangle + G_k^{(\pm)} V |\psi_k^{(\pm)}\rangle \quad \cdots\cdots (20)$$

where

$$G_k^{(\pm)} = \frac{1}{E - H_0 \pm i\epsilon} \quad \cdots\cdots (21).$$

We will now make a slight change of notation. The above Green's function (to be more precise, Green's operator) will now be denoted by $G_0^{(\pm)}(E)$, i.e.,

$$G_0^{(\pm)}(E) \equiv \frac{1}{E - H_0 \pm i\epsilon} \quad \cdots\cdots (22).$$

Since $G_0^{(\pm)}(E)$ is defined in terms of the free Hamiltonian H_0, it is also called free Green's function. We define the Green's function with the full Hamiltonian $H = H_0 + V$ as

$$G^{(\pm)}(E) = \frac{1}{E - H \pm i\epsilon}, \quad \text{------} \quad (23)$$

Now we will derive two identities involving $G^{(\pm)}$ and $G_0^{(\pm)}$. We use the operator identity

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B-A)\frac{1}{B} = \frac{1}{B}(B-A)\frac{1}{A} \qquad (24)$$

Let

$$A = E - H \pm i\epsilon$$

$$B = E - H_0 \pm i\epsilon$$

$$\therefore \quad B - A = V$$

We get

$$\frac{1}{E - H \pm i\epsilon} - \frac{1}{E - H_0 \pm i\epsilon} = \frac{1}{E - H \pm i\epsilon} V \frac{1}{E - H_0 \pm i\epsilon}$$

$$= \frac{1}{E - H_0 \pm i\epsilon} V \frac{1}{E - H \pm i\epsilon}$$

or $$G^{(\pm)}(E) = G_0^{(\pm)}(E) + G^{(\pm)}(E) V G_0^{(\pm)}(E) \quad \text{----} \quad (25)$$

(first identity)

and

$$G^{(\pm)}(E) = G_0^{(\pm)}(E) + G_0^{(\pm)}(E) V G^{(\pm)}(E) \quad \text{----} \quad (26)$$

(2nd identity)

Now, the Lippmann-Schwinger Equation is (Eq. 20)

$$|\psi^{(\pm)}\rangle = |\phi\rangle + G_0^{(\pm)}(E)\,V\,|\psi^{(\pm)}\rangle \quad \ldots\ldots (27)$$

where we have dispensed with the subscript k.

Using the first identity (Eq. 26) we write

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \left(G^{(\pm)} - G^{(\pm)} V G_0^{(\pm)}\right) V |\psi^{(\pm)}\rangle$$

$$= |\phi\rangle + G^{(\pm)} V |\psi^{(\pm)}\rangle - G^{(\pm)} V \underbrace{G_0^{(\pm)} V |\psi^{(\pm)}\rangle}_{\left(|\psi^{(\pm)}\rangle - |\phi\rangle\right)}$$

$$= |\phi\rangle + G^{(\pm)} V |\psi^{(\pm)}\rangle - G^{(\pm)} V \left(|\psi^{(\pm)}\rangle - |\phi\rangle\right)$$

$$= |\phi\rangle + \cancel{G^{(\pm)} V |\psi^{(\pm)}\rangle} - \cancel{G^{(\pm)} V |\psi^{(\pm)}\rangle} + G^{(\pm)} V |\phi\rangle$$

or

$$|\psi^{(\pm)}\rangle = |\phi\rangle + G^{(\pm)} V |\phi\rangle$$

or

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H \pm i\epsilon} V |\phi\rangle. \quad \ldots\ldots (28)$$

This is the formal solution of the Lippmann-Schwinger equation. Even though we have derived a solution of the LS equation, the solution is very difficult to evaluate ~~the~~ ~~[illegible]~~ because of the presence of the full Hamiltonian H in $G^{(\pm)}$.

Transition operator T

Often, in scattering theory, it is convenient to introduce an operator, called the transition operator, ~~[illegible]~~ and, denoted by T, and to express the LS equation in terms of T. To define the transition operator we start with the LS equation (Eq (27)):

$$|\psi\rangle = |\phi\rangle + G_0 V |\psi\rangle. \quad \cdots\cdots (29)$$

We define the operator T such that

$$T|\phi\rangle = V|\psi\rangle \quad \cdots\cdots (30)$$

Therefore, the LS equation, Eq (29), can be written as

$$|\psi\rangle = |\phi\rangle + G_0 T |\phi\rangle \quad \cdots\cdots (31)$$

This equation can be regarded as a formal solution of $|\psi\rangle$ in terms of the operator T.

Now, using LS equation (Eq. (29)) in Eq (30) we get

$$T|\phi\rangle = V\left(|\phi\rangle + G_0 V|\psi\rangle\right)$$

$$= V|\phi\rangle + VG_0 V|\psi\rangle$$

$$= V|\phi\rangle + VG_0 T|\phi\rangle$$

$$= \left(V + VG_0 T\right)|\phi\rangle$$

Hence

$$T = V + VG_0 T. \qquad \text{-------- (32)}$$

This is the integral equation for T. Iterating this equation we get

$$T = V + VG_0 V + VG_0 VG_0 V + VG_0 VG_0 VG_0 V + \cdots \qquad (33)$$

Using (33) we can evaluate T up to different orders in V.

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Next, to get a ~~closed~~ formal solution for T we compare Eq. (28) with Eq. (31). We get

$$G_0 T = G V$$

Using the second identity (Eq. (26)) we find

$$G_0 T = (G_0 + G_0 V G) V$$

$$= G_0 (V + V G V)$$

i.e.,

$$T = V + V G V$$

or,

$$T^{(\pm)} = V + V G^{(\pm)}(E) V \quad \cdots\cdots \quad (34)$$

This equation is the formal solution for the transition operator.

— x —