Scattering theory

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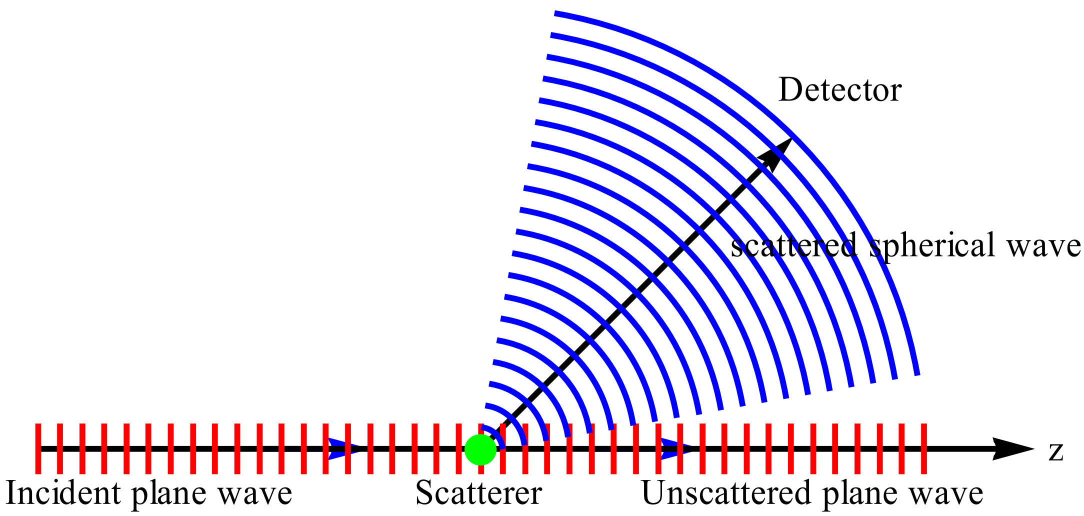
One of the best experimental methods to probe a microscopic structure of the target (system) is to examine the distribution of scattered particles (or wave) from the collision of particles with the target. The experimental results thus obtained are compared with the theory of scattering based on the quantum mechanics. Here we discuss the scattering theory in the quantum mechanics: the Born approximation and (ii) the Lippmann-Schwinger equation. Our understanding on the scattering has been greatly enhanced, thank to these two theories.

Max Born (11 December 1882 – 5 January 1970) was a German born physicist and mathematician who was instrumental in the development of quantum mechanics. He also made contributions to solid-state physics and optics and supervised the work of a number of notable physicists in the 1920s and 30s. Born won the 1954 Nobel Prize in Physics (shared with Walther Bothe).

http://en.wikipedia.org/wiki/Max_Born

Julian Seymour Schwinger (February 12, 1918 – July 16, 1994) was an American theoretical physicist. He is best known for his work on the theory of quantum electrodynamics, in particular for developing a relativistically invariant perturbation theory, and for renormalizing QED to one loop order. Schwinger is recognized as one of the greatest physicists of the twentieth century, responsible for much of modern quantum field theory, including a variational approach, and the equations of motion for quantum fields. He developed the first electroweak model, and the first example of confinement in 1+1 dimensions. He is responsible for the theory of multiple neutrinos, Schwinger terms, and the theory of the spin 3/2 field.

http://en.wikipedia.org/wiki/Julian_Schwinger



1 Green's function in scattering theory

We start with the original Schrödinger equation.

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\boldsymbol{r})+V(\boldsymbol{r})\psi(\boldsymbol{r})=E_k\psi(\boldsymbol{r}),$$

or

$$(\nabla^2+\frac{2\mu}{\hbar^2}E_k)\psi(\boldsymbol{r})=\frac{2\mu}{\hbar^2}V(\boldsymbol{r})\psi(\boldsymbol{r}).$$

under the potential energy $V(\boldsymbol{r})$, where μ is the reduced mass. We assume that

$$E = E_k = \frac{\hbar^2}{2\mu} k^2 ,$$

We put

$$f(\boldsymbol{r}) = -\frac{2\mu}{\hbar^2} V(\boldsymbol{r}) \psi(\boldsymbol{r}) ,$$

Using the operator

$$L_{\mathbf{r}} = \nabla^2 + k^2 .$$

we have the differential equation

$$L_r \psi(\boldsymbol{r}) = (\nabla^2 + k^2) \psi(\boldsymbol{r}) = -f(\boldsymbol{r}) .$$

Suppose that there exists a Green's function $G(\boldsymbol{r})$ such that

$$(\nabla_r{}^2 + k^2) G^{(+)}(\boldsymbol{r}, \boldsymbol{r}') = -\delta(\boldsymbol{r} - \boldsymbol{r}') ,$$

with

$$G^{(+)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{\exp(ik|\boldsymbol{r} - \boldsymbol{r}'|)}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} \qquad \text{(Green function)}$$

We will discuss about the derivation of this Green function later. Then $\psi(\mathbf{r})$ is formally given by

$$\psi^{(+)}(\boldsymbol{r}) = \phi(\boldsymbol{r}) + \int d\boldsymbol{r}' G^{(+)}(\boldsymbol{r}, \boldsymbol{r}') f(\boldsymbol{r}') = \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2} \int d\boldsymbol{r}' \frac{\exp(ik|\boldsymbol{r} - \boldsymbol{r}'|)}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|} V(\boldsymbol{r}') \psi^{(+)}(\boldsymbol{r}') ,$$

where $\phi(\mathbf{r})$ is a solution of the homogeneous equation, satisfying

$$(\nabla^2 + k^2) \phi(\boldsymbol{r}) = 0 ,$$

or

$$\phi(\boldsymbol{r}) = \langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{(2\pi)^{3/2}} \exp(i\boldsymbol{k} \cdot \boldsymbol{r}) , \qquad \text{(plane wave)}$$

with

$$k = |\boldsymbol{k}|$$

Note that

$$(\nabla^2 + k^2)\psi(\boldsymbol{r}) = (\nabla^2 + k^2)\phi(\boldsymbol{r}) + \int d\boldsymbol{r}'(\nabla^2 + k^2)G^{(+)}(\boldsymbol{r},\boldsymbol{r}')f(\boldsymbol{r}')$$
$$= -\int d\boldsymbol{r}'\delta(\boldsymbol{r}-\boldsymbol{r}')f(\boldsymbol{r}')$$
$$= -f(\boldsymbol{r})$$

2. Choice between wave packet and plane wave as an incident wave

((**Sakurai and Napolitano**))

"The reader may wonder here whether our formulation of scattering has anything to do with the motion of a particle bounced by a scattering center. The incident plane wave we have used is infinite in extent in both space and time. In a more realistic situation, we consider a wave packet (a difficult subject!) that approaches the scattering center. After a long time, we have both the original wave packet moving in the original direction, plus a spherical wave front that moves outward, as in Fig. shown here. Actually the use of a plane wave is satisfactory as long as the dimension of the wave packet is much larger than the size of the scatterer)or range of *V*)."

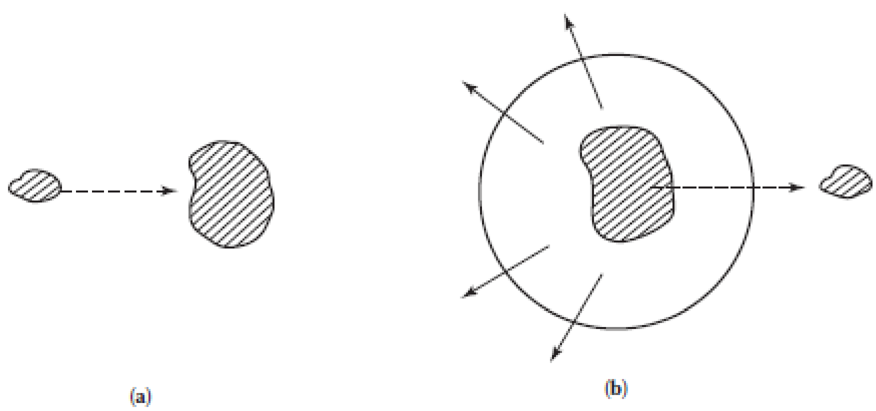


Fig. (a) Incident wave packet (width *w*) approaching scattering center (size *d*) initially. (b) Incident wave packet continuing to move in the original direction plus spherical outgoing wave front (after a long-time duration)

It is considered that the incident wave has a form of wave packet with width *w*, that approaches the scattering center. Nevertheless, we assume that the incident wave is simply expressed by a plane wave. When the size of the target (*d*) is much smaller than the width of the wave packet, the plane wave is the best choice as an incident wave.

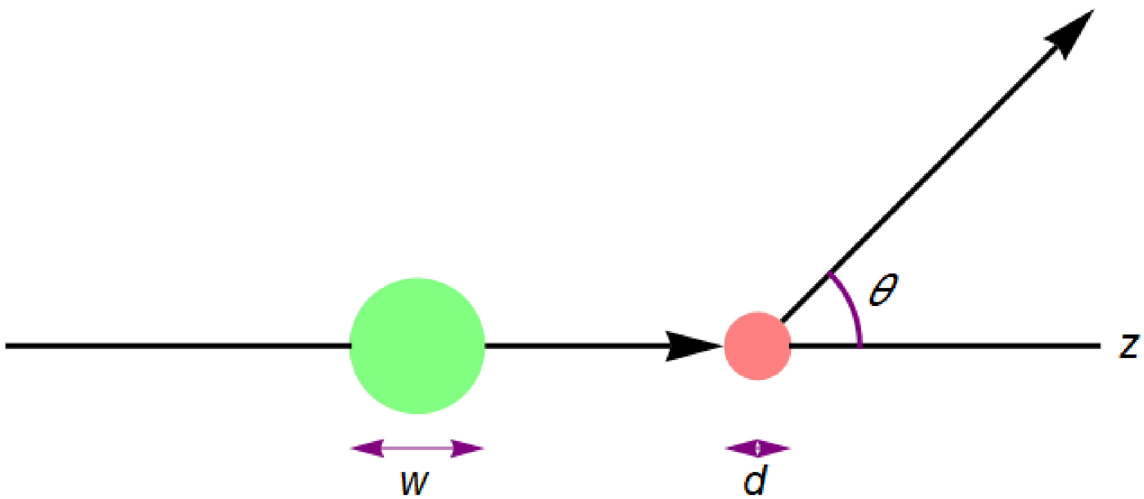


Fig. Before the collision ($t << 0$), the wave packet approaches the target with constant velocity. The size of the target d, the size of wave packet w should satisfy the condition $d << w$.

3. Born approximation

We start with

$$\psi^{(+)}(\boldsymbol{r}) = \phi(\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' \frac{\exp(ik|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}'),$$

$$\phi(\boldsymbol{r}) = \langle r|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad \text{(plane wave).}$$

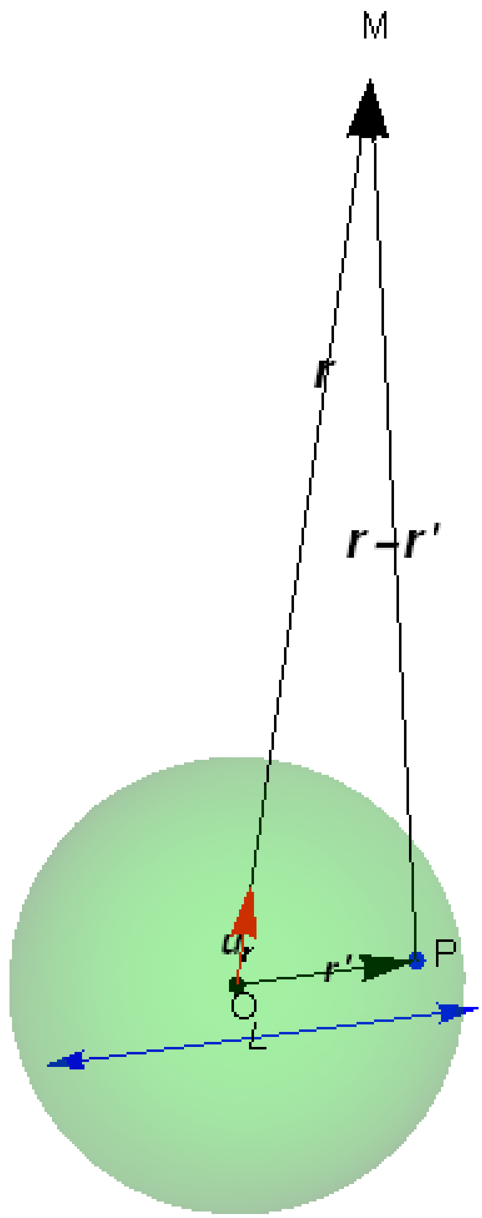


Fig. Vectors r and r' in calculation of scattering amplitude in the first Born approximation. $\boldsymbol{u}_r$ is the unit vector: $\boldsymbol{u}_r = \boldsymbol{r} / r$.

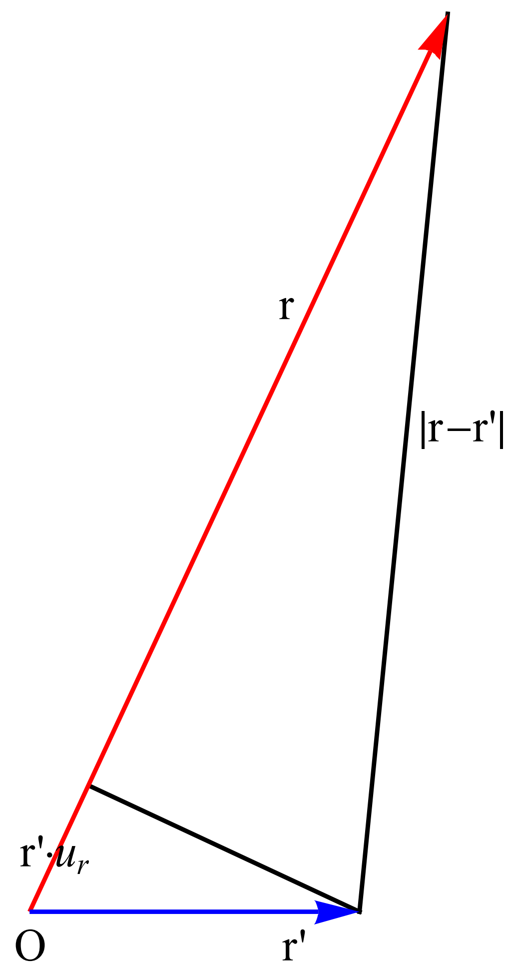


Fig. $\boldsymbol{u}_r = \boldsymbol{e}_r$. $|\boldsymbol{r} - \boldsymbol{r}'| \approx r - \boldsymbol{r}' \cdot \boldsymbol{e}_r$.

Here we consider the case of $\psi^{(+)}(r)$

$$\begin{aligned}
|\boldsymbol{r} - \boldsymbol{r}'|^2 &= (r^2 + r'^2 - 2\boldsymbol{r} \cdot \boldsymbol{r}') \\
&\approx (r^2 - 2\boldsymbol{r} \cdot \boldsymbol{r}') \\
&= r^2 (1 - \frac{2\boldsymbol{r}}{r^2} \cdot \boldsymbol{r}')
\end{aligned}$$

or

$$\left|\boldsymbol{r}-\boldsymbol{r}'\right| \approx r(1-\frac{2\boldsymbol{r}}{r^2}\cdot\boldsymbol{r}')^{1/2}$$

$$= r(1-\frac{\boldsymbol{r}}{r^2}\cdot\boldsymbol{r}')$$

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

$$= r-\boldsymbol{e}_r\cdot\boldsymbol{r}'$$

or

$$\left|\boldsymbol{r}-\boldsymbol{r}'\right| \approx r-\boldsymbol{e}_r\cdot\boldsymbol{r}'$$

$$\boldsymbol{k}' = k\boldsymbol{e}_r$$

$$e^{ik\left|\boldsymbol{r}-\boldsymbol{r}'\right|} \approx e^{ik(r-\boldsymbol{r}'\cdot\boldsymbol{e}_r)} = e^{ikr}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \qquad \text{for large } r.$$

$$\frac{1}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|} \approx \frac{1}{r}$$

Then we have

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')$$

or

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\boldsymbol{k}',\boldsymbol{k})]$$

The first term denotes the original plane wave in propagation direction $\boldsymbol{k}$. The second denotes the term: outgoing spherical wave with amplitude, $f(\boldsymbol{k}',\boldsymbol{k})$,

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{4\pi}(2\pi)^{3/2}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\psi^{(+)}(\boldsymbol{r}')\,.$$

The first Born approximation:

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')e^{i\boldsymbol{k}\cdot\boldsymbol{r}'}$$

$$= -\frac{\mu}{2\pi\hbar^2}\int d\boldsymbol{r}' V(\boldsymbol{r}')e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}'}$$

when $\psi^{(+)}(r)$ is approximated by

$$\psi^{(+)}(r) \approx \frac{1}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} .$$

Note that $f(\boldsymbol{k}',\boldsymbol{k})$ is the Fourier transform of the potential energy with the wave vector $\boldsymbol{Q}$; the scattering vector;

$$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k} .$$

Formally $f(\boldsymbol{k}',\boldsymbol{k})$ can be rewritten as

$$\begin{aligned} f(\boldsymbol{k}',\boldsymbol{k}) &= -\frac{\mu}{2\pi\hbar^2}(2\pi)^3 \langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \\ &= -\frac{4\pi^2\mu}{\hbar^2}\langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle \end{aligned}$$

where

$$\begin{aligned} \langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle &= \int d^3\boldsymbol{r} \langle \boldsymbol{k}'|\boldsymbol{r}\rangle V(\boldsymbol{r}) \langle \boldsymbol{r}|\boldsymbol{k}\rangle \\ &= \frac{1}{(2\pi)^3}\int d^3\boldsymbol{r} e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r}) \end{aligned}$$

with

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) .$$

((**Forward scattering**))

Suppose that $\boldsymbol{k}' = \boldsymbol{k}$ ($\boldsymbol{Q} = 0$) Then we have

$$\begin{aligned} f(0) &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot\boldsymbol{r}'} V(\boldsymbol{r}') e^{i\boldsymbol{k}\cdot\boldsymbol{r}'} \\ &= -\frac{\mu}{2\pi\hbar^2}\int d\boldsymbol{r}' V(\boldsymbol{r}') \end{aligned}$$

Suppose that the attractive potential is a type of square-well

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & r > R \end{cases}$$

Then we have

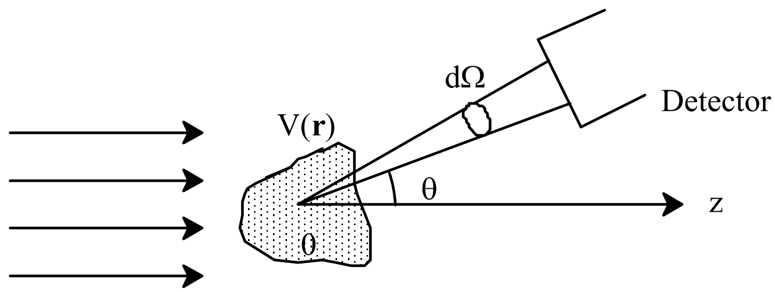
$$f(0) = \frac{2}{3}\frac{\mu V_0}{\hbar^2}R^3 \approx \frac{\mu V_0}{\hbar^2}R^3$$

The total cross section (which is isotropic) is obtained as

$$\sigma = 4\pi |f(0)|^2 = 4\pi \left(\frac{\mu V_0}{\hbar^2}R^3\right)^2 .$$

The units of $f(0)$ is cm, and the units of σ is cm^2.

4. Differential cross section



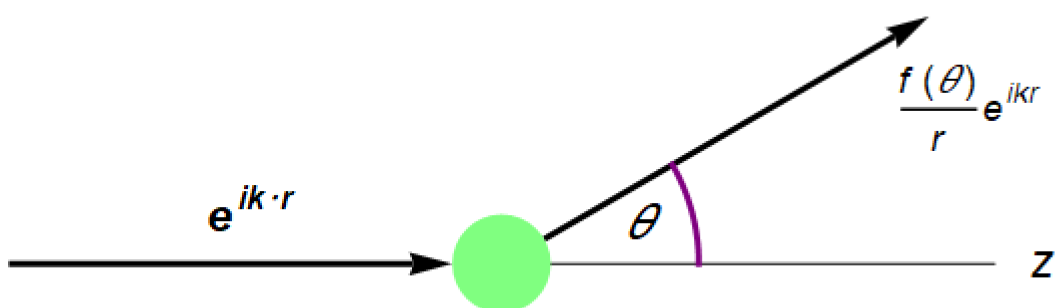


Fig. Incoming plane wave ($e^{i\mathbf{k}\cdot\mathbf{r}}$) and outgoing spherical wave ($\frac{e^{ikr}}{r} f(\theta)$.

We define the differential cross section $\frac{d\sigma}{d\Omega}$ as the number of particles per unit time scattered into an element of solid angle $d\Omega$ divided by the incident flux of particles.

The probability flux associated with a wave function

$$\phi_k(\boldsymbol{r}) = \langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{(2\pi)^{3/2}} e^{ikz},$$

is obtained as

$$N_z = J_z = \frac{\hbar}{2\mu i}[\varphi_k^*(\boldsymbol{r})\frac{\partial}{\partial z}\varphi_k(\boldsymbol{r}) - \varphi_k(\boldsymbol{r})\frac{\partial}{\partial z}\varphi_k^*(\boldsymbol{r})] = \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu} = \frac{1}{(2\pi)^3} v$$

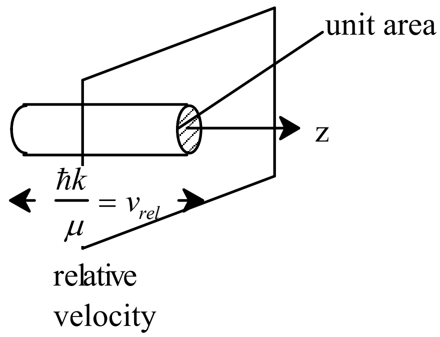


Fig. Probability flux.

$$\text{volume} = \frac{\hbar k}{\mu} \times 1$$

$|e^{ikz}|^2 = 1$ means that there is one particle per unit volume. J_z is the probability flow (probability per unit area per unit time) of the incident beam crossing a unit surface perpendicular to OZ

The probability flux associated with the scattered wave function

$$\chi_r = \frac{1}{(2\pi)^{3/2}} \frac{e^{ikr}}{r} f(\theta) \qquad \text{(spherical wave)}$$

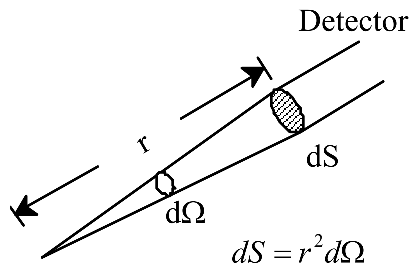
is

$$J_r = \frac{\hbar}{2\mu i}(\chi_r^* \frac{\partial}{\partial r}\chi_r - \chi_r \frac{\partial}{\partial r}\chi_r^*) = \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\frac{|f(\theta)|^2}{r^2}$$

Since $dA = r^2 d\Omega$,

$$\Delta N = J_r dA = \frac{v}{(2\pi)^3}\frac{|f(\theta)|^2}{r^2} r^2 d\Omega = \frac{v}{(2\pi)^3}|f(\theta)|^2 d\Omega$$

where J_r is the probability flow (probability per unit area per unit time)



The differential cross section

$$\frac{d\sigma}{d\Omega} d\Omega = \frac{\Delta N}{N_z} = \left| f(\theta) \right|^2 d\Omega$$

or

$$\frac{\partial \sigma}{\partial \Omega} = \left| f(\theta) \right|^2 .$$

First-order Born amplitude:

$$\begin{aligned} f(\boldsymbol{k}', \boldsymbol{k}) &= -\frac{1}{4\pi} (2\pi)^3 \frac{2\mu}{\hbar^2} \langle \boldsymbol{k}' | V | \boldsymbol{k} \rangle \\ &= -\frac{\mu}{2\pi\hbar^2} \int d^3\boldsymbol{r}' e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} V(\boldsymbol{r}') , \\ &= -\frac{\mu}{2\pi\hbar^2} \int d^3\boldsymbol{r}' e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}} V(\boldsymbol{r}') \end{aligned}$$

which is the Fourier transform of the potential with respect to $\boldsymbol{Q}$, where

$\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}$: scattering wave vector.

$|\boldsymbol{Q}| = Q = 2k \sin\frac{\theta}{2}$ for the elastic scattering.

The Ewald sphere is given by this figure. Note that the scattering angle is θ here. In the case of x-ray and neutron diffraction, we use the scattering angle 2θ, instead of θ.

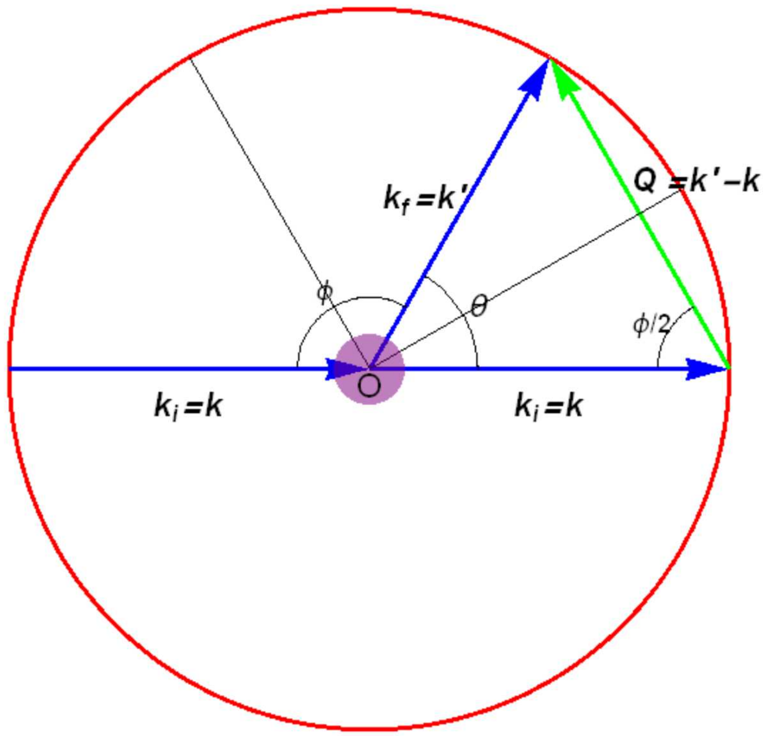


Fig. Ewald sphere for the present system (elastic scattering). $\boldsymbol{k}_{\mathrm{i}} = \boldsymbol{k}$. $\boldsymbol{k}_{\mathrm{f}} = \boldsymbol{k}'$. $\boldsymbol{Q} = \boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ (scattering wave vector). $|\boldsymbol{Q}| = 2k\sin\frac{\theta}{2}$.

((**Ewald sphere**)) **x-ray and neutron scattering**

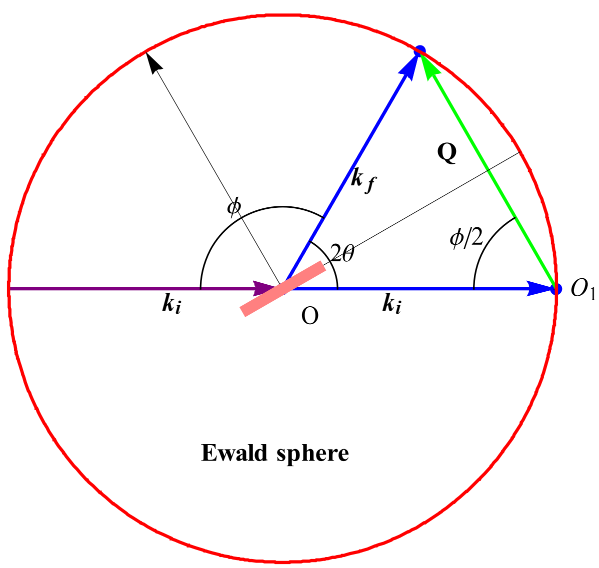


Fig. Ewald sphere used for the x-ray and neutron scattering experiments. $\boldsymbol{k}_{\mathrm{i}} = \boldsymbol{k}$. $\boldsymbol{k}_{\mathrm{f}} = \boldsymbol{k}'$. $\boldsymbol{Q} = \boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ (scattering wave vector). Note that in the conventional x-ray and neutron scattering experiments, we use the angle 2θ, instead of θ for both the x-ray and neutron scattering,

5. Spherical symmetric potential

When the potential energy $V(\boldsymbol{r})$ is dependent only on r, it has a spherical symmetry. For simplicity we assume that θ' is an angle between $\boldsymbol{Q}$ and $\boldsymbol{r}'$.

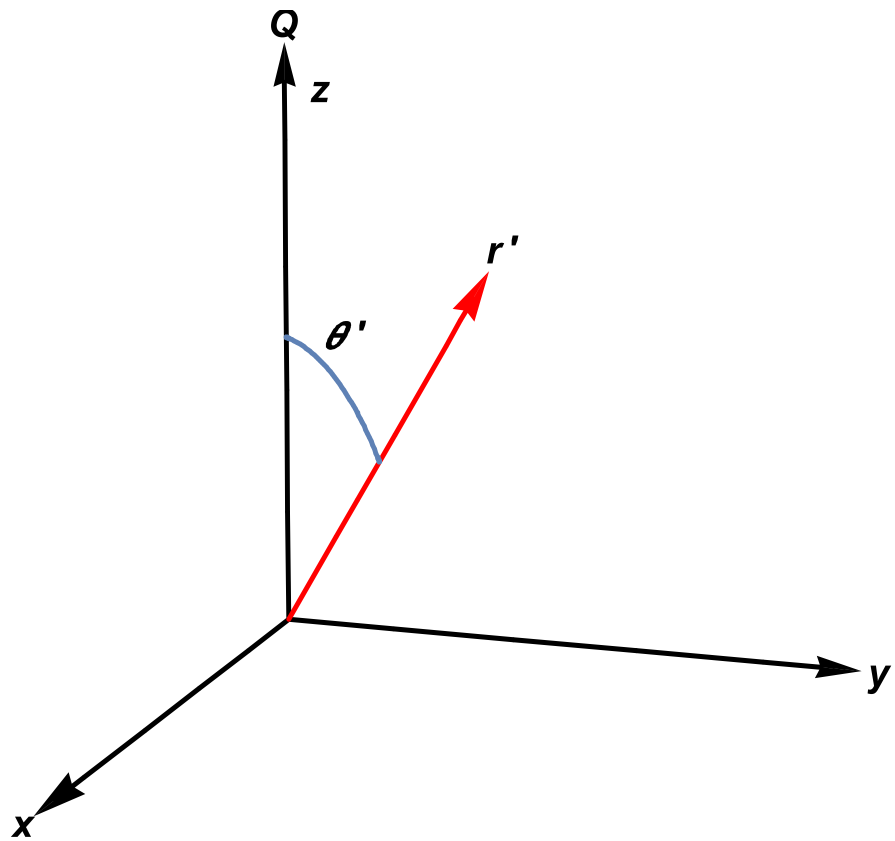
$$\boldsymbol{Q}\cdot\boldsymbol{r}' = Qr'\cos\theta' .$$

We can perform the angular integration over θ'.

$$\begin{aligned} f^{(1)}(\theta) &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}' e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}'}V(\boldsymbol{r}') \\ &= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int_0^\infty dr' \int_0^\pi d\theta' e^{-iQr'\cos\theta'} 2\pi r'^2 \sin\theta' V(r') \\ &= -\frac{\mu}{\hbar^2}\int_0^\infty dr' \int_0^\pi d\theta' e^{-iQr'\cos\theta'} r'^2 \sin\theta' V(r') \end{aligned}$$

Note that

$$\int_0^\pi d\theta' e^{-iQr'\cos\theta'} \sin\theta' = \frac{2}{Qr'}\sin(Qr')$$



Then

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int_0^\infty dr' 2\pi r'^2 V(r')\frac{2}{Qr'}\sin(Qr')$$
$$= -\frac{1}{Q}\frac{2\mu}{\hbar^2}\int_0^\infty dr' r' V(r')\sin(Qr')$$

(spherical symmetry)

Then the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \frac{1}{Q^2}\left(\frac{2\mu}{\hbar^2}\right)^2\left|\int_0^\infty dr' r' V(r')\sin(Qr')\right|^2$$

Then we find that $f^{(1)}(\theta)$ is a function of Q.

$$Q = 2k\sin(\frac{\theta}{2}),$$

where θ is an angle between ***k***' and ***k*** (Ewald's sphere).

6. Low energy soft-sphere scattering

Suppose that

$$V(r) = \begin{cases} V_0 & r \le R \\ 0 & r > R \end{cases}$$

Then we get

$$\begin{aligned} f^{(1)}(\theta) &= -\frac{1}{Q}\frac{2\mu}{\hbar^2}V_0\int_0^R dr' r' \sin(Qr') \\ &= -\frac{1}{Q}\frac{2\mu}{\hbar^2}V_0\frac{\sin(QR) - QR\cos(QR)}{Q^2} \\ &= -\frac{2\mu}{\hbar^2}R^3V_0\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3} \end{aligned}$$

When QR<<1,

$$\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3} \approx \frac{1}{3} - \frac{x^2}{30}.$$

where $x = QR$. Then we have

$$f^{(1)}(\theta) \approx -\frac{2\mu}{\hbar^2}R^3V_0\frac{1}{3} = -\frac{\mu}{2\pi\hbar^2}V_0\left(\frac{4\pi}{3}R^3\right)$$

and

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \left(\frac{2\mu V_0}{3\hbar^2}R^3\right)^2$$

with

$$Q = 2k\sin(\frac{\theta}{2}),$$

We make a plot of $\left|f^{(1)}(Q)\right|^2 / \left|f^{(1)}(Q=0)\right|^2$ as a function QR.

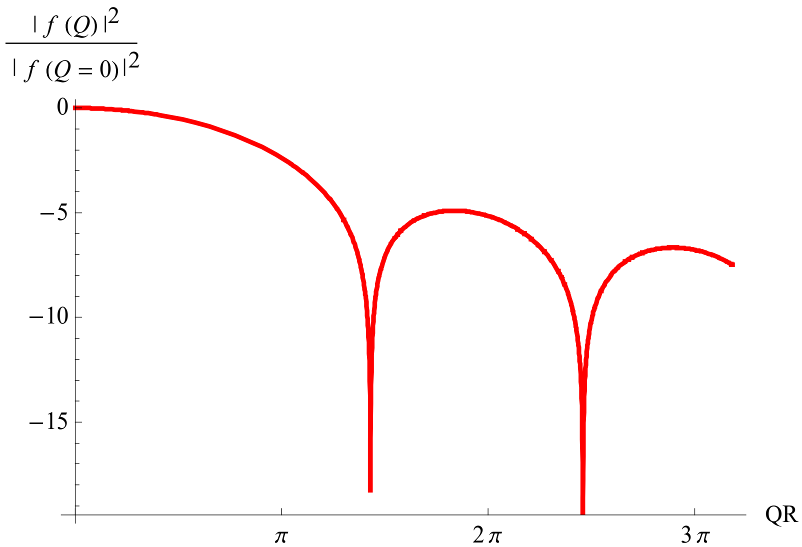


Fig. Semi log plot of $\left|f^{(1)}(Q)\right|^2/\left|f^{(1)}(Q=0)\right|^2$ as a function QR. The value of $\left|f^{(1)}(Q)\right|^2$ becomes zero when QR = 4.49341 and 7.72525.

7. Yukawa potential

Hideki Yukawa (23 January 1907 – 8 September 1981) was a Japanese theoretical physicis-t and the first Japanese Nobel laureate.

http://en.wikipedia.org/wiki/Hideki_Yukawa

The Yukawa potential is given by

$$V(r) = \frac{V_0}{\mu_0 r} e^{-\mu_0 r},$$

where V_0 is independent of *r*. $1/\mu_0$ corresponds to the range of the potential.

$$f^{(1)}(\theta) = -\frac{2\mu}{\hbar^2}\frac{1}{Q}\int_0^\infty dr' r' \frac{V_0}{\mu_0 r'} e^{-\mu_0 r'} \sin(Qr') = -\frac{2\mu}{\hbar^2}\frac{1}{Q}\frac{V_0}{\mu_0}\int_0^\infty dr' e^{-\mu_0 r'} \sin(Qr')$$

Here we use μ_0 for the Yukawa potential in order to avoid the confusion of the reduced mass μ. Note that

$$\int_0^\infty dr' e^{-\mu_0 r'} \sin(Qr') = \frac{Q}{Q^2 + \mu_0^2}, \qquad \text{(Laplace transformation)}$$

or

$$f^{(1)}(\theta) = -\frac{2\mu}{\hbar^2}\frac{V_0}{\mu_0}\frac{1}{Q^2 + \mu_0^2}.$$

Since

$$Q^2 = 4k^2 \sin^2(\frac{\theta}{2}) = 2k^2(1-\cos\theta)$$

so, in the first Born approximation,

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \left(\frac{2\mu V_0}{\mu_0 \hbar^2}\right)^2 \frac{1}{[2k^2(1-\cos\theta) + \mu_0^2]^2}.$$

Note that as $\mu_0 \to 0$, the Yukawa potential is reduced to the Coulomb potential, provided the ratio V_0/μ_0 is fixed.

$$\frac{V_0}{\mu_0} = ZZ'e^2,$$

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \frac{(2\mu)^2 (ZZ'e^2)^2}{\hbar^4}\frac{1}{16k^4 \sin^4(\theta/2)}.$$

Using $E_k = \dfrac{\hbar^2 k^2}{2\mu}$, we have

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$
$$= \left(\frac{ZZ'e^2}{4E_k}\right)^2 \frac{1}{\sin^4(\theta/2)}$$
$$= \left(\frac{ZZ'\alpha(\hbar c)}{4E_k}\right)^2 \frac{1}{\sin^4(\theta/2)}$$

with

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035999084(21)}$$

which is the Rutherford scattering cross section (that can be obtained classically).

8. Validity of the first-order Born approximation

If the Born approximation is to be applicable, $\langle \boldsymbol{r} | \psi^{(+)} \rangle$ should not be too different from $\langle \boldsymbol{r} | \boldsymbol{k} \rangle$ inside the range of potential. The distortion of the incident wave must be small.

$$\langle \boldsymbol{r} | \psi^{(+)} \rangle = \langle \boldsymbol{r} | \boldsymbol{k} \rangle - \frac{2\mu}{\hbar^2} \int d\boldsymbol{r}' \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}') \langle \boldsymbol{r}' | \psi^{(+)} \rangle$$

$\langle \boldsymbol{r} | \psi^{(+)} \rangle \approx \langle \boldsymbol{r} | \boldsymbol{k} \rangle$ at the center of scattering potential at $\boldsymbol{r} = 0$.

$$\left| \frac{2\mu}{\hbar^2} \int d\boldsymbol{r}' \frac{e^{ikr'}}{4\pi r'} V(\boldsymbol{r}') \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}} \right| << \frac{1}{(2\pi)^{3/2}},$$

or

$$\left| \frac{\mu}{2\pi\hbar^2} \int d\boldsymbol{r}' \frac{e^{ikr'}}{r'} V(\boldsymbol{r}') e^{i\boldsymbol{k}\cdot\boldsymbol{r}'} \right| << 1.$$

For spherical potential, we have

$$I = \int d\boldsymbol{r}' \frac{e^{ikr'}}{r'} V(r') e^{i\boldsymbol{k}\cdot\boldsymbol{r}'} = 2\pi \iint dr' r'^2 \sin\theta' d\theta' \frac{e^{ikr'}}{r'} V(r') e^{ikr'\cos\theta'}$$

or

$$I = 2\pi \iint dr' r' e^{ikr'} V(r') \sin\theta' d\theta' e^{ikr'\cos\theta'}$$

$$= 2\pi \int dr' r' e^{ikr'} V(r') \int_0^{\pi} \sin\theta' d\theta' e^{ikr'\cos\theta'}$$

$$= 2\pi \int dr' r' e^{ikr'} V(r') \frac{2}{kr'} \sin(kr')$$

$$= \frac{4\pi}{k} \int dr' e^{ikr'} V(r') \sin(kr')$$

where

$$\int_0^{\pi} \sin\theta' d\theta' e^{ikr'\cos\theta'} = \frac{2}{kr'} \sin(kr')$$

Then we get

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

At $k \to \infty$, the integrand oscillates rapidly. It becomes zero for $r' > 1/k$. Then we have

$$\left| \frac{2\mu}{\hbar^2 k} \int_0^{\infty} dr' e^{ikr'} V(r') \sin(kr') \right| \approx \frac{\mu}{\hbar^2 k} V_0 \int_0^{1/k} dr' kr' \approx \frac{\mu V_0}{\hbar^2 k^2} << 1,$$

or

$$\frac{V_0}{E} << 1.$$

In other words, the Born approximation is applicable only for the scattering of particles with high energy. In the low energy limit, in turn the phase shift analysis is more useful.

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9. Lippmann-Schwinger equation

The **Lippmann–Schwinger equation** (named after Bernard Lippmann and Julian Schwinger) is one of the most used equations to describe particle collisions– or, more precisely, scattering– in quantum mechanics. It may be used in scattering of molecules, atoms, neutrons, photons or any other particles and is important mainly in atomic, molecular, and optical physics, nuclear physics and particle physics, but also for seismic scattering problems in geophysics. It relates the scattered wave function with the interaction that produces the scattering (the scattering potential) and therefore allows calculation of the relevant experimental parameters (scattering amplitude and cross sections).

The Lippmann–Schwinger equation is equivalent to the Schrödinger equation plus the typical boundary conditions for scattering problems. In order to embed the boundary conditions, the Lippmann–Schwinger equation must be written as an integral equation. For scattering problems, the Lippmann–Schwinger equation is often more convenient than the original Schrödinger equation.
(http://en.wikipedia.org/wiki/Lippmann%E2%80%93Schwinger_equation)

B.A. Lippmann and J. Schwinger, *Phys. Rev.* **19**, 469 (1950).

The Hamiltonian $\hat{H}$ of the system is given by

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where H_0 is the Hamiltonian of free particle. Let $|\phi\rangle$ be the eigenket of H_0 with the energy eigenvalue E,

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

The basic Schrödinger equation is

$$\hat{H}|\psi\rangle = (\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle. \tag{1}$$

Both $\hat{H}_0$ and $\hat{H}_0 + \hat{V}$ exhibit continuous energy spectra. We look for a solution to Eq.(1) such that as $V \to 0$, $|\psi\rangle \to |\phi\rangle$, where $|\phi\rangle$ is the solution to the free particle Schrödinger equation with the same energy eigenvalue E.

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

Since $\hat{H}_0|\phi\rangle = E|\phi\rangle$ or $(E - \hat{H}_0)|\phi\rangle = 0$, this can be rewritten as

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

which leads to

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

or

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

The presence of $|\phi\rangle$ is reasonable because $|\psi\rangle$ must reduce to $|\phi\rangle$ as $\hat{V}$ vanishes.

Lippmann-Schwinger equation:

$$|\psi^{(\pm)}\rangle = |\boldsymbol{k}\rangle + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle$$

by making E_k (= $\hbar^2\boldsymbol{k}^2/2\mu$) slightly complex number (ε>0, ε≈0). This can be rewritten as

$$\langle\boldsymbol{r}|\psi^{(\pm)}\rangle = \langle\boldsymbol{r}|\boldsymbol{k}\rangle + \int dr'\langle\boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

where

$$\langle\boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}},$$

and

$$\hat{H}_0|\boldsymbol{k}'\rangle = E_{k'}|\boldsymbol{k}'\rangle,$$

with

$$E_{k'} = \frac{\hbar^2}{2\mu}k'^2.$$

The Green's function is defined by

$$G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}') = -\frac{\hbar^2}{2\mu}\langle\boldsymbol{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\boldsymbol{r}'\rangle = \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}e^{\pm ik|\boldsymbol{r}-\boldsymbol{r}'|}$$

((**Proof**))

$$\begin{aligned} I &= -\frac{\hbar^2}{2\mu}\langle\mathbf{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\mathbf{r}'\rangle \\ &= -\frac{\hbar^2}{2\mu}\int\int d\mathbf{k}'d\mathbf{k}''\langle\mathbf{r}|\mathbf{k}'\rangle(E_k - \frac{\hbar^2}{2\mu}\mathbf{k}'^2 \pm i\varepsilon)^{-1}\langle\mathbf{k}'|\mathbf{k}''\rangle\langle\mathbf{k}''|\mathbf{r}'\rangle \end{aligned}$$

or

$$I=-\frac{\hbar^2}{2\mu}\int\int d\mathbf{k}'d\mathbf{k}''\langle\mathbf{r}|\mathbf{k}'\rangle(E_k-\frac{\hbar^2}{2\mu}\mathbf{k}'^2\pm i\varepsilon)^{-1}\delta(\mathbf{k}'-\mathbf{k}'')\langle\mathbf{k}''|\mathbf{r}'\rangle$$
$$=-\frac{\hbar^2}{2\mu}\int d\mathbf{k}'\langle\mathbf{r}|\mathbf{k}'\rangle(E_k-\frac{\hbar^2}{2\mu}\mathbf{k}'^2\pm i\varepsilon)^{-1}\langle\mathbf{k}'|\mathbf{r}'\rangle$$
$$=-\frac{\hbar^2}{2\mu}\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{E_k-\frac{\hbar^2}{2\mu}\mathbf{k}'^2\pm i\varepsilon}$$

where

$$E_k=\frac{\hbar^2}{2\mu}\boldsymbol{k}^2.$$

Then we have

$$I=-\frac{\hbar^2}{2\mu}\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{\frac{\hbar^2}{2\mu}(\mathbf{k}^2-\mathbf{k}'^2)\pm i\varepsilon}$$
$$=\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{k'^2-(k^2\pm i\varepsilon)}$$

So, we have

$$G_0^{(\pm)}(\boldsymbol{r}-\boldsymbol{r}')=\frac{1}{(2\pi)^3}\int d\boldsymbol{k}'\frac{e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{k'^2-(k^2\pm i\varepsilon)}$$

where $\varepsilon>0$ is infinitesimally small value. In summary, we get

$$\langle\boldsymbol{r}|\psi^{(\pm)}\rangle=\langle\boldsymbol{r}|\boldsymbol{k}\rangle-\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}'G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}')\langle\boldsymbol{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

or

$$\langle\boldsymbol{r}|\psi^{(\pm)}\rangle=\langle\boldsymbol{r}|\boldsymbol{k}\rangle-\frac{2\mu}{\hbar^2}\int d\boldsymbol{r}'G_0^{(\pm)}(\boldsymbol{r},\boldsymbol{r}')V(\boldsymbol{r}')\langle\boldsymbol{r}'|\psi^{(\pm)}\rangle.$$

More conveniently, the Lippmann-Schwinger equation can be rewritten as

$$|\psi^{(\pm)}\rangle=|\boldsymbol{k}\rangle+(E_k-\hat{H}_0\pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle$$

with

$$\hat{G}_0^{(\pm)} = -\frac{\hbar^2}{2\mu}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1},$$

and

$$-\frac{2\mu}{\hbar^2}\hat{G}_0^{(\pm)}\hat{V} = (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}$$

When two operators $\hat{A}$ and $\hat{B}$ are not commutable, we have very useful formula as follows,

$$\frac{1}{\hat{A}} - \frac{1}{\hat{B}} = \frac{1}{\hat{A}}(\hat{B} - \hat{A})\frac{1}{\hat{B}} = \frac{1}{\hat{B}}(\hat{B} - \hat{A})\frac{1}{\hat{A}}, \qquad \text{(formula)}$$

((**Proof**))

$$\begin{aligned}\hat{A}^{-1} - \hat{B}^{-1} &= \hat{A}^{-1}(\hat{1} - \hat{A}\hat{B}^{-1}) \\ &= \hat{A}^{-1}(\hat{B}\hat{B}^{-1} - \hat{A}\hat{B}^{-1}) \\ &= \hat{A}^{-1}(\hat{B} - \hat{A})\hat{B}^{-1}\end{aligned}$$

or

$$\begin{aligned}\hat{A}^{-1} - \hat{B}^{-1} &= \hat{B}^{-1}(\hat{B}\hat{A}^{-1} - \hat{1}) \\ &= \hat{B}^{-1}(\hat{B}\hat{A}^{-1} - \hat{A}\hat{A}^{-1}) \\ &= \hat{B}^{-1}(\hat{B} - \hat{A})\hat{A}^{-1}\end{aligned}$$

We assume that

$$\hat{A} = (E_k - \hat{H}_0 \pm i\varepsilon), \qquad \hat{B} = (E_k - \hat{H} \pm i\varepsilon)$$

$$\hat{A} - \hat{B} = \hat{H} - \hat{H}_0 = \hat{V}$$

Then

$$(E_k - \hat{H}_0 \pm i\varepsilon)^{-1} = (E_k - \hat{H} \pm i\varepsilon)^{-1} - (E_k - \hat{H} \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1},$$

from $\hat{A}^{-1} - \hat{B}^{-1} = \hat{B}^{-1}(\hat{B} - \hat{A})\hat{A}^{-1}$

or

$$(E_k - \hat{H} \pm i\varepsilon)^{-1} = (E_k - \hat{H}_0 \pm i\varepsilon)^{-1} + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}(E_k - \hat{H} \pm i\varepsilon)^{-1}.$$

from $\hat{A}^{-1} - \hat{B}^{-1} = \hat{A}^{-1}(\hat{B} - \hat{A})\hat{B}^{-1}$.

For simplicity, we newly define the two operators by

$$\hat{G}_0(E_k \pm i\varepsilon) = (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}$$

$$\hat{G}(E_k \pm i\varepsilon) = (E_k - \hat{H} \pm i\varepsilon)^{-1}$$

where $\hat{G}_0(E_k + i\varepsilon)$ denotes an outgoing spherical wave and $\hat{G}_0(E_k - i\varepsilon)$ denotes an in-coming spherical wave. We note that

$$\hat{G}_0^{(\pm)} = -\frac{\hbar^2}{2\mu}(E_k - \hat{H}_0 \pm i\varepsilon)^{-1} = -\frac{\hbar^2}{2\mu}\hat{G}_0(E_k \pm i\varepsilon).$$

Then we have

$$\begin{aligned}\hat{G}_0(E_k \pm i\varepsilon) &= \hat{G}(E_k \pm i\varepsilon) - \hat{G}(E_k \pm i\varepsilon)\hat{V}\hat{G}_0(E_k \pm i\varepsilon) \\ &= \hat{G}(E_k \pm i\varepsilon)[1 - \hat{V}\hat{G}_0(E_k \pm i\varepsilon)]\end{aligned}$$

and

$$\begin{aligned}\hat{G}(E_k \pm i\varepsilon) &= \hat{G}_0(E_k \pm i\varepsilon) + \hat{G}_0(E_k \pm i\varepsilon)\hat{V}\hat{G}(E_k \pm i\varepsilon) \\ &= \hat{G}_0(E_k \pm i\varepsilon)[1 + \hat{V}\hat{G}(E_k \pm i\varepsilon)]\end{aligned}$$

Then $\left|\psi^{(\pm)}\right\rangle$ can be rewritten as

$$\begin{aligned}\left|\psi^{(\pm)}\right\rangle &= \left|\mathbf{k}\right\rangle + \hat{G}_0(E_k \pm i\varepsilon)\hat{V}\left|\psi^{(\pm)}\right\rangle \\ &= \left|\mathbf{k}\right\rangle + \hat{G}(E_k \pm i\varepsilon)[\hat{1} - \hat{V}\hat{G}_0(E_k \pm i\varepsilon)]\hat{V}\left|\psi^{(\pm)}\right\rangle \\ &= \left|\mathbf{k}\right\rangle + \hat{G}(E_k \pm i\varepsilon)\hat{V}(\left|\psi^{(\pm)}\right\rangle - \hat{G}_0(E_k \pm i\varepsilon)\hat{V}\left|\psi^{(\pm)}\right\rangle \\ &= \left|\mathbf{k}\right\rangle + \hat{G}(E_k \pm i\varepsilon)\hat{V}\left|\mathbf{k}\right\rangle \\ &= [\hat{1} + \hat{G}(E_k \pm i\varepsilon)\hat{V}]\left|\mathbf{k}\right\rangle\end{aligned}$$

or

$$\left|\psi^{(\pm)}\right\rangle = \left|\boldsymbol{k}\right\rangle + \frac{1}{E_k - \hat{H} \pm i\varepsilon}\hat{V}\left|\boldsymbol{k}\right\rangle.$$

Note that

$$\left|\psi^{(\pm)}\right\rangle = \left|\mathbf{k}\right\rangle + \hat{G}_0(E_k \pm i\varepsilon)^{-1}\hat{V}\left|\psi^{(\pm)}\right\rangle.$$

((**Note**)) **Significance of Lippmann-Schwinger equation**

Translation from S. Sunagawa, Quantum theory of scattering (in Japanese)

The method of Lippmann-Schwinger (LS) was developed after the World War II. Thanks to this method, the theoretical study on the scattering has a significant progress. One of the reasons is that LS equation can be used for a complicated case such that the scattering does not occur due to the potential; that is to say, when the target is a complicated structure consisting of many particles. In this case, the Hamiltonian $\hat{H}_0$ in the propagator $\hat{G}_0^{(\pm)}$ cannot be expressed in simple way, leading to the difficulties in expressing the concrete form, $\hat{G}_0^{(\pm)}$. In the LS equation, $\hat{H}_0$ in $\hat{G}_0^{(\pm)}$ can be replaced by the corresponding Hamiltonian without knowing any knowledge of $\hat{H}_0$. So, the theoretical treatment can be done smoothly. The second reason is that we can also consider the interaction between fields as well as the potential form. In other words, the LS equation can be applied to the quantum field theory.

10. The higher order Born Approximation

From the iteration, $\left|\psi^{(+)}\right\rangle$ can be expressed as

$$\begin{aligned}\left|\psi^{(+)}\right\rangle &= \left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}\left|\psi^{(+)}\right\rangle \\ &= \left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}(\left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}\left|\psi^{(+)}\right\rangle) \\ &= \left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}\left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}\hat{G}_0(E_k + i\varepsilon)\hat{V}\left|\boldsymbol{k}\right\rangle + ...\end{aligned}$$

The Lippmann-Schwinger equation is given by

$$\left|\psi^{(+)}\right\rangle = \left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{V}\left|\psi^{(+)}\right\rangle = \left|\boldsymbol{k}\right\rangle + \hat{G}_0(E_k + i\varepsilon)\hat{T}\left|\boldsymbol{k}\right\rangle,$$

where the transition operator $\hat{T}$ is defined as

$$\hat{V}\left|\psi^{(+)}\right\rangle = \hat{T}\left|\boldsymbol{k}\right\rangle$$

or

$$\hat{T}|\boldsymbol{k}\rangle = \hat{V}|\psi^{(+)}\rangle = \hat{V}|\boldsymbol{k}\rangle + \hat{V}\hat{G}_0(E_k + i\varepsilon)\hat{T}|\boldsymbol{k}\rangle$$

This is supposed to hold for any $|\boldsymbol{k}\rangle$ taken to be any plane-wave state.

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0(E_k + i\varepsilon)\hat{T}\,.$$

The scattering amplitude $f(\boldsymbol{k}',\boldsymbol{k})$ can now be written as

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\boldsymbol{k}'|\hat{V}|\psi^{(+)}\rangle = -\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle.$$

((**Note**)) **Derivation of the scattering amplitude**

$$|\psi^{(\pm)}\rangle = |\boldsymbol{k}\rangle + (E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle$$

$$\begin{aligned}\langle\mathbf{r}|\psi^{(\pm)}\rangle &= \langle\mathbf{r}|\mathbf{k}\rangle + \langle\mathbf{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}\hat{V}|\psi^{(\pm)}\rangle \\ &= \langle\mathbf{r}|\mathbf{k}\rangle + \int d\mathbf{r}'\langle\mathbf{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\mathbf{r}'\rangle\langle\mathbf{r}'|\hat{V}|\psi^{(\pm)}\rangle \\ &= \langle\mathbf{r}|\mathbf{k}\rangle + \int d\mathbf{r}'\langle\mathbf{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\mathbf{r}'\rangle V(\mathbf{r}')\langle\mathbf{r}'|\psi^{(\pm)}\rangle\end{aligned}$$

Here we use the expressions

$$\begin{aligned}G^{(\pm)}(\mathbf{r},\mathbf{r}') &= -\frac{\hbar^2}{2\mu}\langle\mathbf{r}|(E_k - \hat{H}_0 \pm i\varepsilon)^{-1}|\mathbf{r}'\rangle \\ &= \frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}e^{ik|\mathbf{r}-\mathbf{r}'|}\end{aligned}$$

and

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

Thus, we have

$$\langle\mathbf{r}|\psi^{(\pm)}\rangle = \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2\mu}{\hbar^2}\frac{1}{4\pi}\int d\mathbf{r}'\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\langle\mathbf{r}'|\psi^{(\pm)}\rangle$$

Using the approximation

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}=\frac{1}{r}e^{ikr}e^{-i\mathbf{k}'\cdot\mathbf{r}'}$$

we get

$$\begin{aligned}\langle\mathbf{r}|\psi^{(\pm)}\rangle&=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}}-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int d\mathbf{r}'e^{i\mathbf{k}'\cdot\mathbf{r}'}V(\mathbf{r}')\langle\mathbf{r}'|\psi^{(\pm)}\rangle\\&=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}}-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}\int d\mathbf{r}'(2\pi)^{3/2}\langle\mathbf{k}'|\mathbf{r}'\rangle\langle\mathbf{r}'|\hat{V}|\psi^{(\pm)}\rangle\\&=\frac{1}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{r}}-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}\frac{e^{ikr}}{r}(2\pi)^3\langle\mathbf{k}'|\hat{V}|\psi^{(\pm)}\rangle]\end{aligned}$$

So that, we have the scattering amplitude as

$$\begin{aligned}f(\mathbf{k}',\mathbf{k})&=-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\mathbf{k}'|\hat{V}|\psi^{(\pm)}\rangle\\&=-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\mathbf{k}'|\hat{T}|\mathbf{k}\rangle\end{aligned}$$

since $\hat{V}|\psi^{(\pm)}\rangle=\hat{T}|\mathbf{k}\rangle$.

Using the iteration, we have the Dyson equation

$$\hat{T}=\hat{V}+\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{T}=\hat{V}+\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}+\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}+...$$

Correspondingly, we can expand $f(\boldsymbol{k}',\boldsymbol{k})$ as follows:

$$f(\boldsymbol{k}',\boldsymbol{k})=f^{(1)}(\boldsymbol{k}',\boldsymbol{k})+f^{(2)}(\boldsymbol{k}',\boldsymbol{k})+f^{(3)}(\boldsymbol{k}',\boldsymbol{k})+.......$$

with

$$f^{(1)}(\boldsymbol{k}',\boldsymbol{k})=-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle,$$

$$f^{(2)}(\boldsymbol{k}',\boldsymbol{k})=-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\boldsymbol{k}'|\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}|\boldsymbol{k}\rangle,$$

$$f^{(3)}(\boldsymbol{k}',\boldsymbol{k})=-\frac{2\mu}{\hbar^2}\frac{1}{4\pi}(2\pi)^3\langle\boldsymbol{k}'|\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}\hat{G}_0(E_k+i\varepsilon)\hat{V}|\boldsymbol{k}\rangle.$$

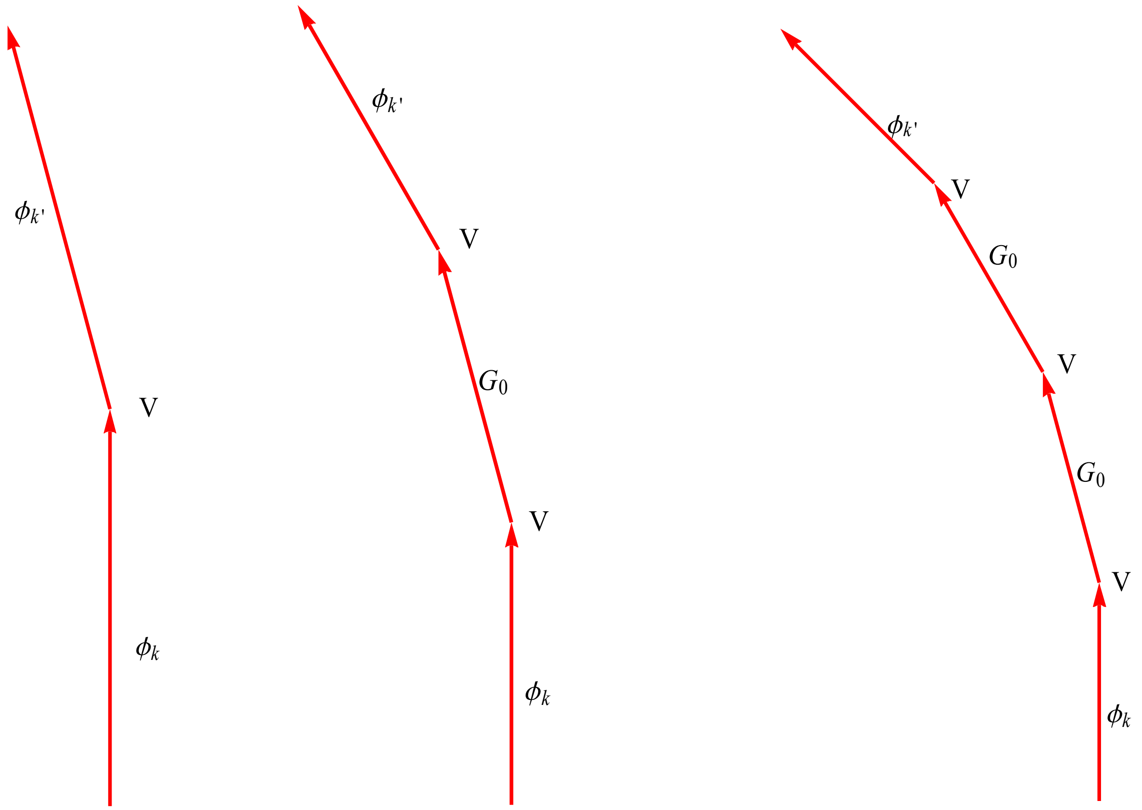

Fig. Feynman diagram. First order, 2nd order, and 3rd order Born approximations. $\phi_k = |\boldsymbol{k}\rangle$ is the initial state of the incoming particle and $\phi_{k'} = |\boldsymbol{k}'\rangle$ is the final state of the incoming particle. $\hat{V}$ is the interaction. (a) $\hat{V}$. (b) $\hat{V}G_0\hat{V}$, and (c) $\hat{V}G_0\hat{V}G_0\hat{V}$.

11. Optical Theorem

The scattering amplitude and the total cross section are related by the identity

$$\mathrm{Im}[f(\theta = 0)] = \frac{k}{4\pi}\sigma_{tot},$$

where

$f(\theta = 0) = f(\boldsymbol{k}, \boldsymbol{k})$: scattering in the forward direction.

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega.$$

This formula is known as the optical theorem, and holds for collisions in general.

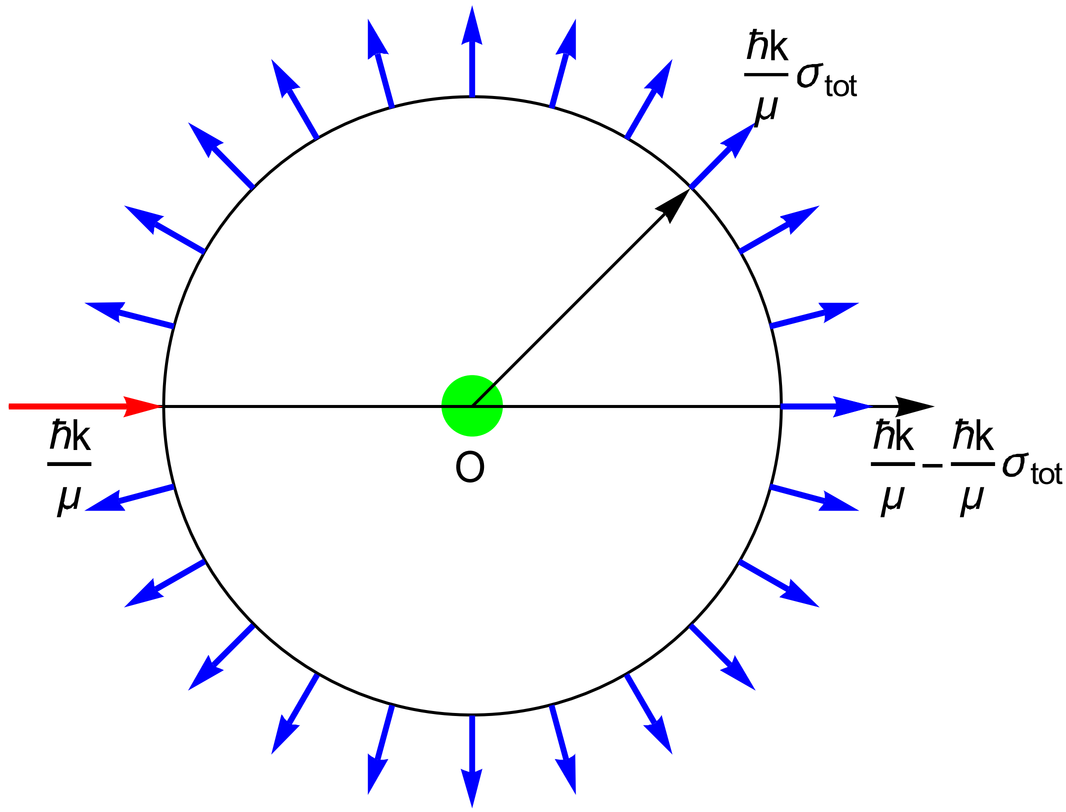

Fig. Optical theorem. The intensity of the incident wave is $\hbar k/\mu$. The intensity of the forward wave is $(\hbar k/\mu)-(4\pi\hbar/\mu)\,\mathrm{Im}[f(0)]$. The waves with the total intensity $(4\pi\hbar/\mu)\,\mathrm{Im}[f(0)]=(\hbar k/\mu)\sigma_{tot}$ is scattered for all the directions, as the scattering spherical waves. Note that a multiplication factor $1/(2\pi)^3$ is required for the expression of probability current.

((**Proof**))

$$\begin{aligned}\mathrm{Im}[f(\boldsymbol{k},\boldsymbol{k})] &= -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle\boldsymbol{k}|\hat{T}|\boldsymbol{k}\rangle] \\ &= -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle\boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle]\end{aligned}$$

$$|\psi^{(+)}\rangle=|\boldsymbol{k}\rangle+\hat{G}_0(E_k+i\varepsilon)\hat{V}|\psi^{(+)}\rangle,$$

or

$$|\boldsymbol{k}\rangle=|\psi^{(+)}\rangle-\hat{G}_0(E_k+i\varepsilon)\hat{V}|\psi^{(+)}\rangle,$$

Hermitian conjugate:

$$\langle \boldsymbol{k}| = \langle \psi^{(+)}| - \langle \psi^{(+)}|\hat{V}\hat{G}_0(E_k - i\varepsilon)$$
.

where

$$[\hat{G}_0(E_k + i\varepsilon)]^+ = \hat{G}_0(E_k - i\varepsilon)\,.$$

Then

$$\begin{aligned}\mathrm{Im}[\langle \mathbf{k}|\hat{V}|\psi^{(+)}\rangle] &= \mathrm{Im}[\{\langle \psi^{(+)}| - \langle \psi^{(+)}|\hat{V}\hat{G}_0(E_k - i\varepsilon)\}\hat{V}|\psi^{(+)}\rangle \\ &= \mathrm{Im}[\langle \psi^{(+)}|\hat{V}|\psi^{(+)}\rangle] - \mathrm{Im}[\langle \psi^{(+)}|\hat{V}\hat{G}_0(E_k - i\varepsilon)\hat{V}|\psi^{(+)}\rangle\,.\end{aligned}$$

Now we use the well-known relation

$$\begin{aligned}\hat{G}_0(E_k - i\varepsilon) &= \left(\frac{1}{E_k - \hat{H}_0 - i\varepsilon}\right) \\ &= [P\left(\frac{1}{E_k - \hat{H}_0}\right) + i\pi\delta(E_k - \hat{H}_0)]\end{aligned}$$

Then

$$\begin{aligned}\mathrm{Im}[\langle \mathbf{k}|\hat{V}|\psi^{(+)}\rangle &= [\mathrm{Im}\langle \psi^{(+)}|\hat{V}|\psi^{(+)}\rangle] - [\mathrm{Im}\langle \psi^{(+)}|\hat{V}P\left(\frac{1}{E - \hat{H}_0}\right)\hat{V}|\psi^{(+)}\rangle \\ &\quad + \mathrm{Im}\langle \psi^{(+)}|\hat{V}i\pi\delta(E - \hat{H}_0)\hat{V}|\psi^{(+)}\rangle]\end{aligned}$$

The first two terms of this equation vanish because of the Hermitian operators of $\hat{V}$ and

$$\hat{V}P\left(\frac{1}{E - \hat{H}_0}\right)\hat{V}\,.$$

Therefore, we have

$$\begin{aligned}\mathrm{Im}[\langle \mathbf{k}|\hat{V}|\psi^{(+)}\rangle &= -\pi\,\langle \psi^{(+)}|\hat{V}\delta(E_k - \hat{H}_0)\hat{V}|\psi^{(+)}\rangle \\ &= -\pi\,\langle \mathbf{k}|\hat{T}^+\delta(E - \hat{H}_0)\hat{T}|\mathbf{k}\rangle\end{aligned}$$

or

$$\mathrm{Im}[\langle \mathbf{k}|\hat{V}|\psi^{(+)}\rangle = -\pi\int d\mathbf{k}'\langle \mathbf{k}|\hat{T}^{+}|\mathbf{k}'\rangle\langle \mathbf{k}'|\hat{T}|\mathbf{k}\rangle \delta(E_k - \frac{\hbar^2 k'^2}{2\mu})$$

$$= -\pi\int d\mathbf{k}'\left|\langle \mathbf{k}'|\hat{T}|\mathbf{k}\rangle\right|^2 \delta(E_k - \frac{\hbar^2 k'^2}{2\mu})$$

$$\delta(E_k - \frac{\hbar^2 k'^2}{2\mu}) = \delta(\frac{\hbar^2 k^2}{2\mu} - \frac{\hbar^2 k'^2}{2\mu})$$

$$= \delta[\frac{\hbar^2}{2\mu}(k^2 - k'^2)]$$

$$= \delta[\frac{\hbar^2}{2\mu}(k+k')(k-k'))]$$

$$= \delta[\frac{k\hbar^2}{\mu}(k-k')]$$

or

$$\delta(E - \frac{\hbar^2 k'^2}{2\mu}) = \frac{\mu}{k\hbar^2}\delta(k-k')$$

So that,

$$\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle = -\pi\frac{\mu}{k\hbar^2}\iint dk' k'^2\, d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2 \delta(k-k')$$

$$= -\pi\frac{\mu k}{\hbar^2}\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

We note that

$$\mathrm{Im}[f(\theta=0)] = -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}\mathrm{Im}[\langle \boldsymbol{k}|\hat{V}|\psi^{(+)}\rangle]$$

$$= -\frac{1}{4\pi}(2\pi)^3\frac{2\mu}{\hbar^2}(-\frac{\pi\mu k}{\hbar^2})\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

$$= \frac{k}{4\pi}\frac{16\pi^4\mu^2}{\hbar^4}\int d\Omega'\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2]$$

Since

$$\frac{d\sigma}{d\Omega'} = |f(\boldsymbol{k}',\boldsymbol{k})|^2$$
$$= \frac{1}{16\pi^2}(2\pi)^6 \frac{4\mu^2}{\hbar^4}\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2,$$
$$= \frac{16\pi^4\mu^2}{\hbar^4}\left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

and

$$\sigma_{tot} = \int d\Omega' \frac{d\sigma}{d\Omega'} = \frac{16\pi^4\mu^2}{\hbar^4}\int d\Omega' \left|\langle \boldsymbol{k}'|\hat{T}|\boldsymbol{k}\rangle\right|^2$$

Then we obtain

$$\mathrm{Im}[f(\theta = 0)] = \frac{k}{4\pi}\sigma_{tot}.$$

((**Note**)) **The violation of optical theorem (E. Merzbacher)**

The first Born approximation violates the optical theorem. It can be remedied by including the second Born approximation for the forward scattering amplitude.

12. Probability Current

Here we discuss the Probability current for the three cases.

$$\mathbf{J}(\mathbf{r}) = \frac{1}{\mu}\mathrm{Re}[\psi(\mathbf{r})^* \mathbf{p}\,\psi(\mathbf{r})]$$
$$= \frac{\hbar}{2i\mu}[\psi(\mathbf{r})^*\nabla\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla\psi^*(\mathbf{r})]$$

For simplicity, we use the wave function

(a) In-coming plane wave

When we use

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

we get the probability current as

$$\mathbf{J}_1 = \mathbf{e}_r \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\cos\theta .$$

(b) Outgoing spherical wave

When we use the wave function

$$\psi_{sc}^{(+)} = \frac{1}{(2\pi)^{3/2}} \frac{1}{r} e^{ikr} f(\theta),$$

we get the probability current

$$\mathbf{J}_2 = \frac{\hbar k}{(2\pi)^3 \mu r^2} \left| f(\theta) \right|^2 \mathbf{e}_r .$$

(c) Outgoing wave with spherical wave and plane wave propagating the forward direction

For the wave function

$$\psi_{out}^{(+)} = \frac{1}{(2\pi)^{3/2}} [e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{1}{r} e^{ikr} f(\theta)]$$

We get the $\mathbf{e}_r$ -component of $\mathbf{J}(\mathbf{r})$ as the probability current

$$\mathbf{e}_r \frac{1}{(2\pi)^3} \frac{\hbar k}{\mu} \cos\theta \qquad \text{(plane wave as independent source)}$$

$$\mathbf{e}_r \frac{1}{(2\pi)^3} \frac{\hbar k}{r^2 \mu} \left| f(\theta) \right|^2 \qquad \text{(spherical wave as independent source)}$$

$$\mathbf{e}_r \frac{1}{2(2\pi)^3} \frac{\hbar k}{\mu r} (1+\cos\theta)[f(\theta) e^{ikr(1-\cos\theta)} + f^*(\theta) e^{-ikr(1-\cos\theta)}]$$

$$+i\mathbf{e}_r \frac{1}{2(2\pi)^3} \frac{\hbar}{\mu r^2} [f(\theta) e^{ikr(1-\cos\theta)} - f^*(\theta) e^{-ikr(1-\cos\theta)}]$$

The first term $\mathbf{e}_r \frac{1}{(2\pi)^3} \frac{\hbar k}{\mu} \cos\theta$ yields null after integration over the sphere.

$$\frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\int_0^\pi 2\pi r^2 \sin\theta\cos\theta d\theta = \frac{1}{(2\pi)^2}\frac{\hbar k}{\mu}r^2\int_0^\pi \sin\theta\cos\theta d\theta$$
$$= \frac{1}{(2\pi)^2}\frac{\hbar k}{2\mu}\int_0^\pi \sin(2\theta) d\theta$$
$$= 0$$

The second $\mathbf{e}_r \frac{1}{(2\pi)^3}\frac{\hbar k}{r^2\mu}|f(\theta)|^2$:

$$\frac{1}{(2\pi)^3}\frac{\hbar k}{r^2\mu}\int |f(\theta)|^2 r^2 d\Omega = \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\int |f(\theta)|^2 d\Omega$$
$$= \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\int \frac{\partial\sigma}{\partial\Omega} d\Omega$$
$$= \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\sigma_{tot}$$

The third and the fourth terms are the interference ones;

$$J_r^{in}(\theta) = \frac{1}{2(2\pi)^3}\frac{\hbar k}{\mu r}(1+\cos\theta)[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

In the limit of $\theta \to 0$ (forward scattering),

$$J_r^{in}(\theta) \simeq \frac{1}{(2\pi)^3}\frac{\hbar k}{\mu r}[f(0)e^{ikr(1-\cos\theta)} + f^*(0)e^{-ikr(1-\cos\theta)}]$$

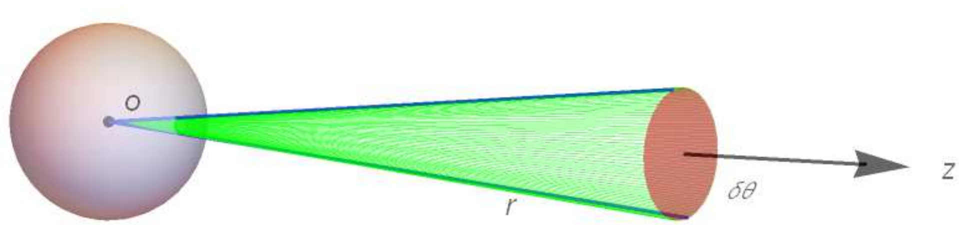

Fig. The forward scattering.

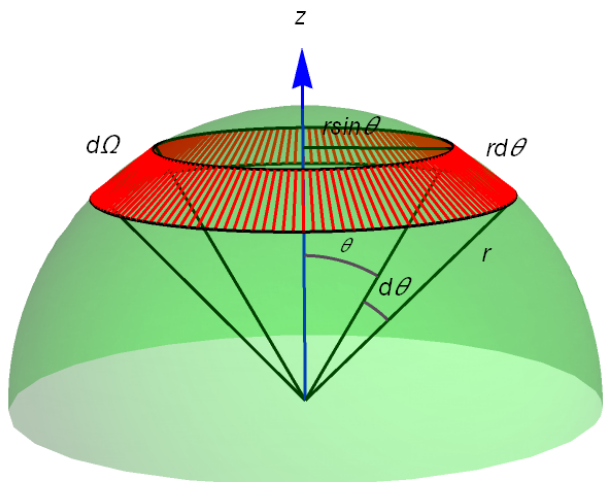

Fig. Surface area contributing to the forward scattering.

The scattering intensity for $0 < \theta < \delta\theta$ ($\delta\theta \simeq 0$) is given by

$$
\begin{aligned}
I &= \int_0^{\delta\theta} 2\pi r^2 \sin\theta d\theta J_r(\theta) \\
&= \frac{1}{(2\pi)^2}\frac{\hbar k r}{\mu}\int_0^{\delta\theta} \sin\theta d\theta [f(0)e^{ikr(1-\cos\theta)} + f^*(0)e^{-ikr(1-\cos\theta)}] \\
&= \frac{1}{(2\pi)^2}\frac{\hbar k r}{\mu}[f(0)\frac{e^{ikr(1-\cos\theta)}}{ikr} - f^*(0)\frac{e^{-ikr(1-\cos\theta)}}{ikr}]_0^{\delta\theta} \\
&= \frac{1}{(2\pi)^2}\frac{\hbar k r}{\mu}\frac{1}{ikr}\{f(0)[e^{ikr(1-\cos\delta\theta)} - 1] - f^*(0)[e^{-ikr(1-\cos\delta\theta)} - 1]]
\end{aligned}
$$

In the limit of $r \to \infty$ but with $\delta\theta \neq 0$, the exponential terms $e^{ikr(1-\cos\delta\theta)}$ and $e^{-ikr(1-\cos\delta\theta)}$ tend to zero because of strong oscillation for the slightest change of *k*.

$$
\begin{aligned}
I &= \frac{1}{(2\pi)^2}\frac{\hbar k r}{\mu}\frac{1}{ikr}[-f(0) + f^*(0)] \\
&= \frac{1}{(2\pi)^2}\frac{\hbar k r}{\mu}\frac{1}{ikr}(-2i)\,\mathrm{Im}[f(0)] \\
&= -\frac{\hbar}{2\pi^2\mu}\mathrm{Im}[f(0)]
\end{aligned}
$$

where

$$\frac{f(0)-f^*(0)}{2i}=\mathrm{Im}\, f(0),$$

Thus, we have the scattering intensity for the forward scattering (the scattering intensity behind the target) is

$$\frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}-\frac{\hbar}{2\pi^2\mu}\mathrm{Im}[f(0)]=\frac{1}{(2\pi)^3}\{\frac{\hbar k}{\mu}-4\pi\frac{\hbar}{\mu}\mathrm{Im}[f(0)]\}$$

From the relation

$$\frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}=\frac{1}{(2\pi)^3}\{\frac{\hbar k}{\mu}-4\pi\frac{\hbar}{\mu}\mathrm{Im}[f(0)]\}+\frac{1}{(2\pi)^3}\frac{\hbar k}{\mu}\sigma_{tot}$$

or

$$\frac{\hbar k}{\mu}=\frac{\hbar k}{\mu}-4\pi\frac{\hbar}{\mu}\mathrm{Im}[f(0)]+\frac{\hbar k}{\mu}\sigma_{tot}$$

leading to the optical theorem

$$\mathrm{Im}[f(0)]=\frac{k}{4\pi}\sigma_{tot}$$

We now evaluation of $\nabla\cdot\mathbf{J}$

(a) Incoming plane wave

$$\psi_{in}(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad \nabla\cdot\mathbf{J}_{in}=0$$

(b) Outgoing spherical wave

$$\psi_{sc}^{(+)}=\frac{1}{(2\pi)^{3/2}}\frac{1}{r}e^{ikr}f(\theta) \qquad \nabla\cdot\mathbf{J}_{sc}=\frac{2\hbar k}{(2\pi)^3\mu r}\left|f(\theta)\right|^2+O(\frac{1}{r^2})$$

(c) Outgoing wave with spherical wave and plane wave propagating the forward direction

$$\psi_{out}{}^{(+)} = \frac{1}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{1}{r}e^{ikr} f(\theta)]$$

$$\nabla\cdot\mathbf{J}_{out} = \frac{-i\hbar\cot\theta}{2(2\pi)^3\mu r^3}[\frac{\partial f(\theta)}{\partial\theta}e^{ikr(1-\cos\theta)} - \frac{\partial f^*(\theta)}{\partial\theta}e^{-ikr(1-\cos\theta)}]$$
$$\frac{-i\hbar}{2(2\pi)^3\mu r^3}[\frac{\partial^2 f(\theta)}{\partial\theta^2}e^{ikr(1-\cos\theta)} - \frac{\partial^2 f^*(\theta)}{\partial\theta^2}e^{-ikr(1-\cos\theta)}]$$

which is on the order of $1/r^3$. In the limit of $r\rightarrow\infty$, we get

$$\nabla\cdot\mathbf{J}_{out} = 0$$

as well as $\nabla\cdot\mathbf{J}_{in} = 0$

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((**Mathematica**))

Evaluation of the probability current density

```
Clear["Global`"];
Gra := Grad[#, {r, θ, ϕ}, "Spherical"] &;
Diva := Div[#, {r, θ, ϕ}, "Spherical"] &;
```

ψ1: Wave function of scattered wave

ψ1c: Complex conjugate of Wave function of scattered wave

```
ψ1[r_, θ_] :=
  1/(2 π)^(3/2) (Exp[ⅈ k r Cos[θ]] + 1/r Exp[ⅈ k r] f1[θ]);
ψ1c[r_, θ_] :=
  1/(2 π)^(3/2) (Exp[-ⅈ k r Cos[θ]] +
     1/r Exp[-ⅈ k r] f1c[θ]);
```

$$\psi 1[r\_, \theta\_] := \frac{1}{(2\pi)^{3/2}}\left(\mathrm{Exp}[i\, k\, r\, \mathrm{Cos}[\theta]] + \frac{1}{r}\mathrm{Exp}[i\, k\, r]\, f1[\theta]\right);$$

$$\psi 1c[r\_, \theta\_] := \frac{1}{(2\pi)^{3/2}}\left(\mathrm{Exp}[-i\, k\, r\, \mathrm{Cos}[\theta]] + \frac{1}{r}\mathrm{Exp}[-i\, k\, r]\, f1c[\theta]\right);$$

Evaluation of probability current density

```
J1 =
  ħ/(2 μ ⅈ) (ψ1c[r, θ] × Gra[ψ1[r, θ]] -
      ψ1[r, θ] × Gra[ψ1c[r, θ]]) //
   FullSimplify;
```

---

e_r component of J1

```
Expand[ J1[[1]]]
```

$$\frac{k\hbar\,\mathrm{Cos}[\theta]}{8\pi^3\mu}+\frac{i\,e^{2ikr-ikr(1+\mathrm{Cos}[\theta])}\,\hbar\,\mathrm{f1}[\theta]}{16\pi^3 r^2\mu}+\frac{e^{2ikr-ikr(1+\mathrm{Cos}[\theta])}\,k\hbar\,\mathrm{f1}[\theta]}{16\pi^3 r\mu}+\frac{e^{2ikr-ikr(1+\mathrm{Cos}[\theta])}\,k\hbar\,\mathrm{Cos}[\theta]\,\mathrm{f1}[\theta]}{16\pi^3 r\mu}-\frac{i\,e^{2ikr\,\mathrm{Cos}[\theta]-ikr(1+\mathrm{Cos}[\theta])}\,\hbar\,\mathrm{f1c}[\theta]}{16\pi^3 r^2\mu}+\frac{e^{2ikr\,\mathrm{Cos}[\theta]-ikr(1+\mathrm{Cos}[\theta])}\,k\hbar\,\mathrm{f1c}[\theta]}{16\pi^3 r\mu}+$$

$$\frac{e^{2 i k r \text{Cos}[\theta] - i k r (1+\text{Cos}[\theta])} k \hbar \text{Cos}[\theta] \, \text{f1c}[\theta]}{16 \pi^3 r \mu} +$$

$$\frac{k \hbar \, \text{f1}[\theta] \times \text{f1c}[\theta]}{8 \pi^3 r^2 \mu}$$

e_ϕ component of J1

Expand[J1[[2]]]

$$-\frac{k \hbar \text{Sin}[\theta]}{8 \pi^3 \mu} -$$

$$\frac{e^{-i k r (-1+\text{Cos}[\theta])} k \hbar \, \text{f1}[\theta] \, \text{Sin}[\theta]}{16 \pi^3 r \mu} -$$

$$\frac{e^{i k r (-1+\text{Cos}[\theta])} k \hbar \, \text{f1c}[\theta] \, \text{Sin}[\theta]}{16 \pi^3 r \mu} -$$

$$\frac{i \, e^{-i k r (-1+\text{Cos}[\theta])} \hbar \, \text{f1}'[\theta]}{16 \pi^3 r^2 \mu} -$$

$$\frac{i \hbar \, \text{f1c}[\theta] \, \text{f1}'[\theta]}{16 \pi^3 r^3 \mu} +$$

$$\frac{i \, e^{i k r (-1+\text{Cos}[\theta])} \hbar \, \text{f1c}'[\theta]}{16 \pi^3 r^2 \mu} +$$

$$\frac{i \hbar \, \text{f1}[\theta] \, \text{f1c}'[\theta]}{16 \pi^3 r^3 \mu}$$

13. Summary

Comparison between the partial wave approximation (low-energy scattering) ans high-energy scattering (Born approximation).

(i) Although the partial wave expansion is "straightforward", when the energy of incident particles is high (or the potential weak), many partial waves contribute. In this case, it is convenient to switch to a different formalism, the Born approximation.

(ii) At low energies, the partial wave expansion is dominated by small orbital angular momentum.

14. Example

Here we discuss the Problem 6-1 of Sakurai amd Napolitano.

6-1

6.1 The Lippmann-Schwinger formalism can also be applied to a *one*-dimensional transmission-reflection problem with a finite-range potential, $V(x) \neq 0$ for $0 < |x| < a$ only.

(a) Suppose we have an incident wave coming from the left: $\langle x|\phi\rangle = e^{ikx}/\sqrt{2\pi}$. How must we handle the singular $1/(E - H_0)$ operator if we are to have a transmitted wave only for $x > a$ and a reflected wave and the original wave for $x < -a$? Is the $E \rightarrow E + i\varepsilon$ prescription still correct? Obtain an expression for the appropriate Green's function and write an integral equation for $\langle x|\psi^{(+)}\rangle$.

(b) Consider the special case of an attractive δ-function potential

$$V = -\left(\frac{\gamma\hbar^2}{2m}\right)\delta(x) \quad (\gamma > 0).$$

Solve the integral equation to obtain the transmission and reflection amplitudes. Check your results with Gottfried 1966, p. 52.

(c) The one-dimensional δ-function potential with $\gamma > 0$ admits one (and only one) bound state for any value of γ. Show that the transmission and reflection amplitudes you computed have bound-state poles at the expected positions when k is regarded as a complex variable.

((**Solution**))

We use the Lippmann-Schwinger equation

$$\left|\psi^{(+)}\right\rangle = |\phi\rangle + \frac{1}{E - \hat{H}_0 + i\varepsilon}\hat{V}\left|\psi^{(+)}\right\rangle$$

Green function:

$$
\begin{aligned}
G_+(x,x') &= \frac{\hbar^2}{2m}\langle x|\frac{1}{E-\hat{H}_0+i\varepsilon}|x'\rangle \\
&= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}dp'\int_{-\infty}^{\infty}dp''\langle x|p'\rangle\langle p'|\frac{1}{E-\hat{H}_0+i\varepsilon}|p''\rangle\langle p''|x'\rangle \\
&= \frac{\hbar^2}{2m}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp'\int_{-\infty}^{\infty}dp''e^{\frac{ip'x}{\hbar}}\frac{1}{E-\frac{p'^2}{2m}+i\varepsilon}\langle p'|p''\rangle e^{\frac{-ip''x'}{\hbar}} \\
&= \frac{\hbar^2}{2m}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp'e^{\frac{ip'(x-x')}{\hbar}}\frac{1}{E-\frac{p'^2}{2m}+i\varepsilon}
\end{aligned}
$$

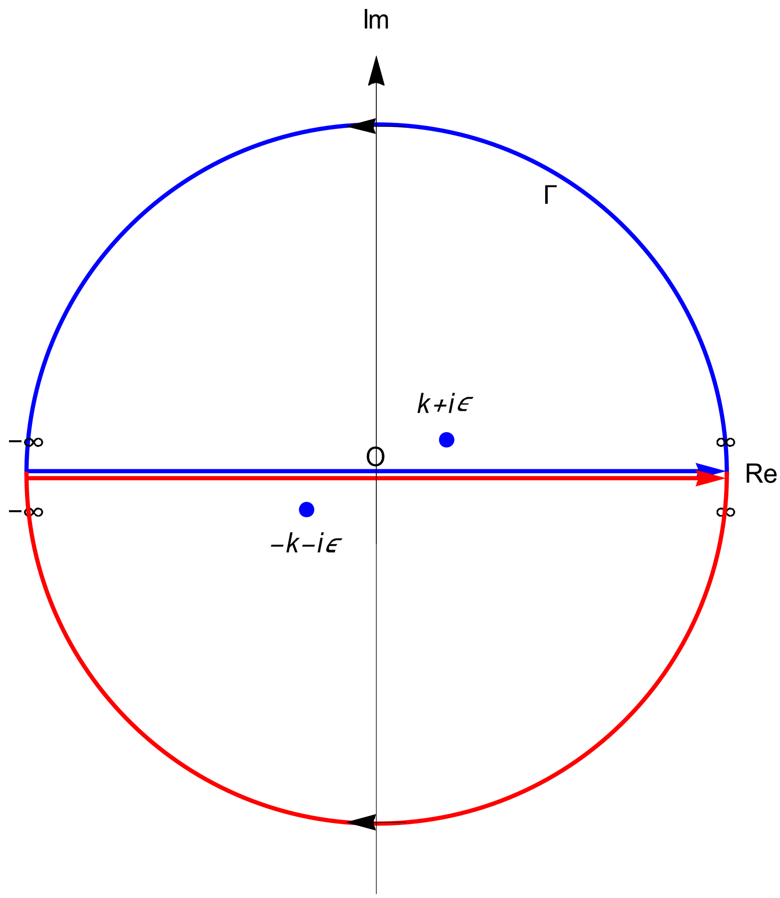
where

$$
\langle x|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ip'x}{\hbar}}, \qquad \langle p'|p''\rangle = \delta_{p',p''}
$$

Here we put

$$
E = \frac{\hbar^2k^2}{2m}, \qquad p' = \hbar k'
$$

$$
G_+(x,x') = -\frac{1}{2\pi}\int_{-\infty}^{\infty}dk'\frac{e^{ik(x-x')}}{k'^2-k^2-i\varepsilon}
$$



$$k' = \pm(k^2 + i\varepsilon)^{1/2}$$
$$= \pm k(1 + \frac{i\varepsilon}{k^2})^{1/2}$$
$$= \pm k(1 + \frac{i\varepsilon}{2k^2})$$
$$= \pm(k + \frac{i\varepsilon}{2k})$$
$$= \pm(k + i\varepsilon)$$

((**Jordan's lemma, residue theorem**))

The integrand has poles in the complex *k*-plane at

$$k' = k + i\varepsilon, \qquad \text{and} \qquad k' = -(k + i\varepsilon)$$

When $x > x'$, we take the path in the upper plane. When $x < x'$, we take the path in the lower plane.

(i) For $x > x'$,

$$G_+(x,x') = -\frac{1}{2\pi} 2\pi i \operatorname{Res}(k' = k + i\varepsilon)$$
$$= -i \frac{e^{ik(x-x')}}{2k}$$

(ii) For $x < x'$,

$$G_+(x,x') = -\frac{1}{2\pi}(-2\pi i) \operatorname{Res}(k' = -k - i\varepsilon)$$
$$= -i \frac{e^{-ik(x-x')}}{2k}$$

Combining Eqs.(1) and (2),

$$G_+(x,x') = -\frac{i}{2k} e^{ik|x-x'|}$$

The Lippmann-Schwinger equation for $\left\langle x \middle| \psi^{(+)} \right\rangle$;

$$\left\langle x \middle| \psi^{(+)} \right\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} - \frac{2m}{\hbar^2} \int_{-\infty}^{\infty} dx' \frac{i}{2k} e^{ik|x-x'|} V(x') \left\langle x' \middle| \psi^{(+)} \right\rangle$$

(b)

$$V = -\frac{\gamma\hbar^2}{2m}\delta(x) \qquad (\gamma > 0).$$

$$\left\langle x \middle| \psi^{(+)} \right\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} - \frac{2m}{\hbar^2} \int_{-\infty}^{\infty} dx' \frac{i}{2k} e^{ik|x-x'|} [-\frac{\gamma\hbar^2}{2m}\delta(x')] \left\langle x' \middle| \psi^{(+)} \right\rangle$$
$$= \frac{1}{\sqrt{2\pi}} e^{ikx} + \gamma \int_{-\infty}^{\infty} dx' \frac{i}{2k} e^{ik|x-x'|} \delta(x')] \left\langle x' \middle| \psi^{(+)} \right\rangle$$
$$= \frac{1}{\sqrt{2\pi}} e^{ikx} + \frac{i\gamma}{2k} e^{ik|x|} \left\langle 0 \middle| \psi^{(+)} \right\rangle$$

When $x = 0$,

$$\left\langle 0 \middle| \psi^{(+)} \right\rangle = \frac{1}{\sqrt{2\pi}} + \gamma \frac{i}{2k} \left\langle 0 \middle| \psi^{(+)} \right\rangle$$

or

$$\langle 0|\psi^{(+)}\rangle = \frac{1}{\sqrt{2\pi}}\frac{1}{1-\frac{i\gamma}{2k}}$$

Then we get

$$\langle x|\psi^{(+)}\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx} + \frac{1}{\sqrt{2\pi}}\frac{\frac{i\gamma}{2k}}{1-\frac{i\gamma}{2k}}e^{ik|x|}$$

For $x>0$

$$\langle x|\psi^{(+)}\rangle = \frac{1}{\sqrt{2\pi}}(\frac{1}{1-\frac{i\gamma}{2k}})e^{ikx}$$

For $x<0$

$$\langle x|\psi^{(+)}\rangle = \frac{1}{\sqrt{2\pi}}[e^{ikx} + \frac{\frac{i\gamma}{2k}}{1-\frac{i\gamma}{2k}}e^{-ikx}]$$

T: probability
R: probability of reflection

$$T = \frac{1}{1+\left(\frac{\gamma}{2k}\right)^2}, \qquad R = 1-T = \frac{\left(\frac{\gamma}{2k}\right)^2}{1+\left(\frac{\gamma}{2k}\right)^2}$$

(c)
The wave function of bound state

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

with

$$V(x) = -\frac{\gamma\hbar^2}{2m}\delta(x)$$

For $x \neq 0$, $\quad V(x) = 0$.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

For $E = -|E| < 0$ (bound state)

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m|E|}{\hbar^2}\psi(x) = \kappa^2\psi(x)$$

The solution of this equation is

$$\psi(x) = Ae^{-\kappa|x|}$$

where

$$|E| = \frac{\hbar^2\kappa^2}{2m}$$

Note that $\psi(x)$ is continuous at $x = 0$, but $d\psi(x)/dx$ is not continuous.

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2}{dx^2}\psi(x)dx - \frac{\gamma\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = -\int_{-\varepsilon}^{\varepsilon}\frac{\hbar^2\kappa^2}{2m}\psi(x)dx$$

$$[\frac{d}{dx}\psi(x)]_{-\varepsilon}^{\varepsilon} = -\gamma\psi(0)$$

leading to the relation

$$\kappa = \frac{\gamma}{2}.$$

Therefore the wave function of the bound state is

$$\psi(x) = \sqrt{\frac{\gamma}{2}}e^{-\gamma|x|/2}$$

The value of k corresponding to the bound state is $k = \frac{i\gamma}{2}$.

$$T = \frac{1}{1+\left(\frac{\gamma}{2k}\right)^2} = \frac{1}{(i+\frac{\gamma}{2k})(-i+\frac{\gamma}{2k})}$$

$$R = \frac{\left(\frac{\gamma}{2k}\right)^2}{1+\left(\frac{\gamma}{2k}\right)^2} = \frac{\left(\frac{\gamma}{2k}\right)^2}{(i+\frac{\gamma}{2k})(-i+\frac{\gamma}{2k})}$$

T and *R* has a pole of $k = \frac{i\gamma}{2}$

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APPENDIX - I

Free particle wave function ψ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi = E_k\psi ,$$

where *m* is the mass of particle,

$$E_k = \frac{\hbar^2 k^2}{2\mu} ,$$

is the energy of the particle, and *k* is the wave number. This equation can be rewritten as

$$(\nabla^2 + k^2)\psi = 0 .$$

This equation is solved in a formal way as

$$\psi = \varphi_{k\ell m}(r,\theta,\phi) = \langle r\theta\phi | k\ell m \rangle$$

$$\frac{1}{2\mu}(p_r{}^2 + \frac{\boldsymbol{L}^2}{r^2})\varphi_{k\ell m}(r,\theta,\phi) = E_k \varphi_{k\ell m}(r,\theta,\phi)$$

(separation variables), where $\boldsymbol{L}$ is the angular momentum:

$$\varphi_{k\ell m}(r,\theta,\phi) = R_{k\ell}(r) Y_{\ell m}(\theta,\phi)$$

with

$$\boldsymbol{L}^2 Y_{\ell m}(\theta,\phi) = \hbar^2 \ell(\ell+1) Y_{\ell m}(\theta,\phi)$$

Since $p_r = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r} r$, we have

$$p_r{}^2 R_{k\ell}(r) = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r} r(\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r} r) R_{k\ell}(r) = -\hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)]$$

or

$$-\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)] + \frac{1}{r^2}\ell(\ell+1)R_{k\ell}(r) = k^2 R_{k\ell}(r)$$

or

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)] + [k^2 - \frac{1}{r^2}\ell(\ell+1)]R_{k\ell}(r) = 0.$$

In the limit of $r \to\infty$, we have

$$\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)] + k^2[rR_{k\ell}(r)] = 0.$$

Then we get

$$R_{kl} = \frac{e^{\pm ikr}}{r} \qquad \text{(outgoing and incoming spherical waves)}$$

APPENDIX II

For the potential

$$V(r) = V_0 R\delta(r - R)$$

Calculate in Born approximation the quantities $f(\theta)$ and $\frac{d\sigma}{d\Omega}$. Specify the limits of validity of your calculation for both high- and low-energy scattering, respectively..
((**Schaum, Quantum Mechanics**))

(a)

$$f^{(1)}(\theta) = -\frac{1}{Q}\frac{2\mu}{\hbar^2}\int_0^\infty dr' r' V(r') \sin(Qr')$$
$$= -\frac{1}{Q}\frac{2\mu}{\hbar^2}\int_0^\infty dr' r' V_0 R\delta(r' - R) \sin(Qr').$$
$$= -\frac{2\mu V_0 R^2}{\hbar^2 Q}\sin(QR)$$

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 = \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 \frac{\sin^2(QR)}{Q^2 R^2}$$

where

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

Validity of the Born approximation

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

or

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

for the potential with the spherical symmetry. In the present case

$$\left|V_0 R\int_0^\infty dr' (e^{2ikr'} - 1)\delta(r' - R)\right| << \frac{\hbar^2 k}{\mu}$$

or

$$V_0 R \frac{2\mu}{\hbar^2 k}\sin(kR) << 1$$

(i) In the limit of *kR*<<1 (low energy limit),

$$V_0 R \frac{2\mu}{\hbar^2 k}\sin(kR) \approx V_0 R^2 \frac{2\mu}{\hbar^2} << 1 .$$

(ii) For high energies,

$$V_0 R \frac{2\mu}{\hbar^2 k}\sin(kR) << 1$$

APPENDIX III The $i\varepsilon$ prescription

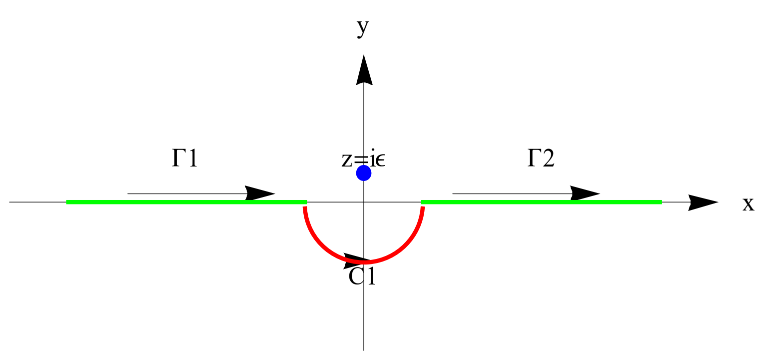
We derive the formula

$$\frac{1}{x \mp i\varepsilon} = P\frac{1}{x} \pm i\pi\delta(x) ,$$

where ε ($\rightarrow$0) is a positive infinitesimally small quantity.

(1) Case-I

$$I_1 = \lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} \frac{f(x)}{x - i\varepsilon} dx$$



Since the only singularity near the real axis is $z = i\varepsilon$, we make the following deformation of the contour without changing the value of I. The contour runs along the real axis (the path Γ1) and goes around counterclockwise, below the origin in a semicircle (C1), and resumes along the real axis (the path Γ2).

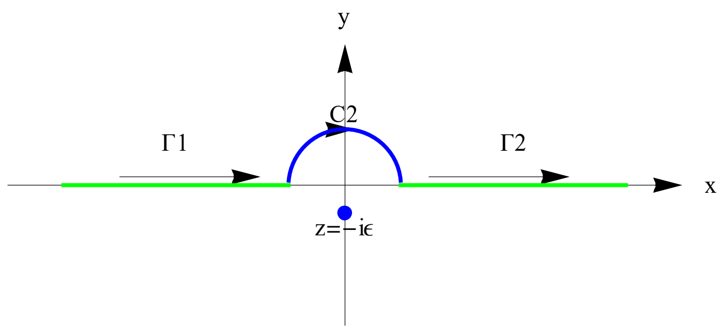
$$I_1 = \int_{\Gamma 1} \frac{f(x)}{x} dx + \int_{C1} \frac{f(z)}{z} dz + \int_{\Gamma 2} \frac{f(x)}{x} dx$$
$$= P\int_{-\infty}^{\infty} \frac{f(x)}{x} dx + \pi i \operatorname{Re} s(z=0)$$
$$= P\int_{-\infty}^{\infty} \frac{f(x)}{x} dx + \pi i f(0)$$

or

$$\frac{1}{x - i\varepsilon} = P\frac{1}{x} + i\pi\delta(x).$$

(2) Case-II

$$I_2 = \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} \frac{f(x)}{x + i\varepsilon} dx$$



Since the only singularity near the real axis is $z = -i\varepsilon$, we make the following deformation of the contour without changing the value of I_2 The contour runs along the real axis (the path $\Gamma 1$) and goes around clockwise, above the origin in a semicircle (C2), and resumes along the real axis (the path $\Gamma 2$).

$$I_2 = \int_{\Gamma 1} \frac{f(x)}{x} dx + \int_{C2} \frac{f(z)}{z} dz + \int_{\Gamma 2} \frac{f(x)}{x} dx$$
$$= P\int_{-\infty}^{\infty} \frac{f(x)}{x} dx - \pi i \operatorname{Re} s(z=0)$$
$$= P\int_{-\infty}^{\infty} \frac{f(x)}{x} dx - \pi i f(0)$$

or

$$\frac{1}{x+i\varepsilon} = P\frac{1}{x} - i\pi\delta(x)$$

APPENDIX IV Plane wave form

There are two-types of wave functions depending on the size of space.

(a) Plane wave in the finite space

For the plane wave in the cube with the size L^3, , the wave function can be expressed by

$$\psi(\boldsymbol{r}) = Ce^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{L^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{V^{1/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

where $k_x = \frac{2\pi}{L}n_x$, $k_y = \frac{2\pi}{L}n_y$, $k_z = \frac{2\pi}{L}n_y$, and the volume of the system is L^3.

The constant C can be determined as

$$1 = \int_V d\boldsymbol{r}\left|\psi(\boldsymbol{r})\right|^2 = \left|C\right|^2 \int_V d\boldsymbol{r} = \left|C\right|^2 L^3,$$

or

$$C = \frac{1}{L^{3/2}}.$$

(b) Plane wave in the free space

For the plane wave in the free space, , the wave function can be expressed by

$$\psi(\boldsymbol{r}) = \frac{1}{(2\pi\hbar)^{3/2}}e^{\frac{i\boldsymbol{p}\cdot\boldsymbol{r}}{\hbar}}, \qquad \text{or} \qquad \psi(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

where $\boldsymbol{p}$ $(=\hbar\boldsymbol{k})$ is a continuous momentum.

$$\langle\boldsymbol{r}|\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \frac{\hbar}{i}\nabla\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \boldsymbol{p}\langle\boldsymbol{r}|\boldsymbol{p}\rangle$$

leading to

$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = C'\exp(\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r})$$

Using the property of Dirac delta function, we get

$$
\begin{aligned}
\langle \boldsymbol{r} | \boldsymbol{r}' \rangle &= \delta(\boldsymbol{r} - \boldsymbol{r}') \\
&= \int d\boldsymbol{p} \langle \boldsymbol{r} | \boldsymbol{p} \rangle \langle \boldsymbol{p} | \boldsymbol{r}' \rangle \\
&= |C'|^2 \int d\boldsymbol{p} \exp[\frac{i}{\hbar} \boldsymbol{p} \cdot (\boldsymbol{r} - \boldsymbol{r}')] \\
&= |C'|^2 (2\pi)^3 \delta[\frac{1}{\hbar} (\boldsymbol{r} - \boldsymbol{r}')] \\
&= |C'|^2 (2\pi\hbar)^3 \delta(\boldsymbol{r} - \boldsymbol{r}')
\end{aligned}
$$

leading to

$$
C' = \frac{1}{(2\pi\hbar)^{3/2}}
$$