Chapter 18 Scattering in Quantum Mechanics
Application of 3D Green's function

Masatsugu Sei Suzuki
Department of Physics
SUNY at Binghamton
(Date: November 16, 2010)

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

18.1 Green's function in scattering theory

We return to the original Schrödinger equation.

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

or

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

We assume that

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

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

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

$$L_{\mathbf{r}}\psi(\mathbf{r})=(\nabla^2+k^2)\psi(\mathbf{r})=-f(\mathbf{r})$$

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

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

with

$$G(\mathbf{r},\mathbf{r}') = \frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|} .$$

Then $\psi(\mathbf{r})$ is formally given by

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

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

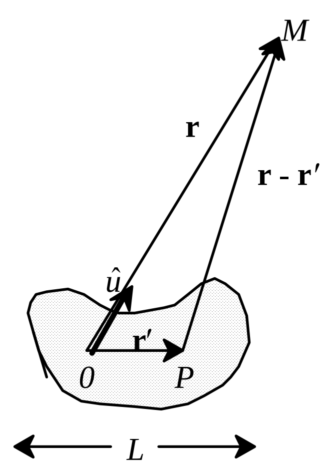
$$(\nabla^2 + k^2)\phi(\mathbf{r}) = 0 ,$$

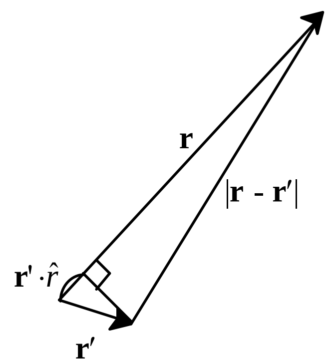
$$\phi(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{(2\pi)^{3/2}}\exp(i\mathbf{k}\cdot\mathbf{r}) , \qquad \text{(plane wave)}$$

with

$$k = |\mathbf{k}|$$

18.2 Born approximation





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

$$|\mathbf{r}-\mathbf{r}'| = r - \mathbf{r}'\cdot\mathbf{e}_r$$

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

$$e^{ik|\mathbf{r}-\mathbf{r}'|} \approx e^{ik(r-\mathbf{r}'\cdot\mathbf{e}_r)} = e^{ikr}e^{-i\mathbf{k}'\cdot\mathbf{r}'}$$ for large r.

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} \approx \frac{1}{r}$$

Then we have

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

or

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

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

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

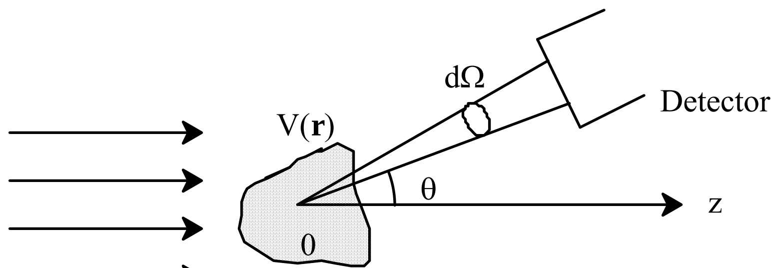
The first Born approximation:

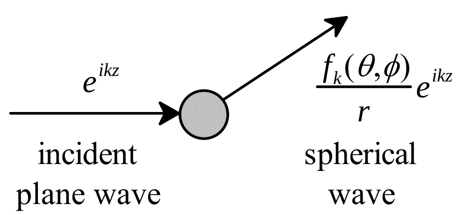
$$f(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d\mathbf{r}' e^{-i\mathbf{k}'\cdot\mathbf{r}'} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'}$$

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

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

18.3 Differential cross section





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 particle flux associated with a wave function

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

is obtained as

$$N_z = J_z = \frac{\hbar}{2mi}[\phi_k^*(\mathbf{r})\frac{\partial}{\partial z}\phi_k(\mathbf{r}) - \phi_k(\mathbf{r})\frac{\partial}{\partial z}\phi_k^*(\mathbf{r})] = \frac{1}{(2\pi)^{3/2}}\frac{\hbar k}{m} = \frac{v}{(2\pi)^{3/2}}$$

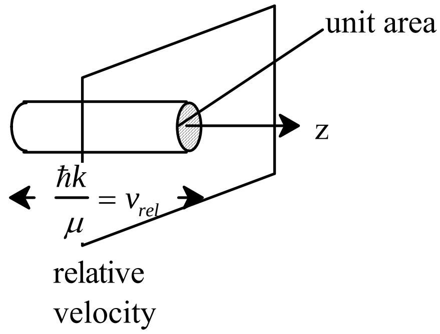


Fig. Note that $\mu = m$ in this figure.

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

$\left| e^{ikz} \right|^2 = 1$ means that there is one particle per unit volume. J_z is the incident flux (number of particles) of the incident beam crossing a unit surface perpendicular to OZ per unit time.

The flux associated with the scattered wave function

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

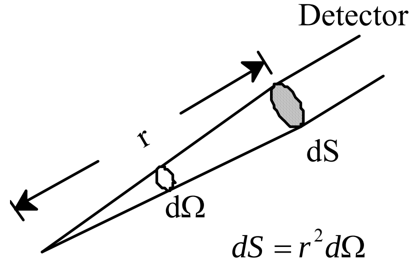
is

$$J_r = \frac{\hbar}{2mi}(\chi_r^* \frac{\partial}{\partial r}\chi_r - \chi_r \frac{\partial}{\partial r}\chi_r^*) = \frac{1}{(2\pi)^{3/2}} \frac{\hbar k}{m} \frac{\left| f(\theta) \right|^2}{r^2}$$

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

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

(the number of particles which strike the opening of the detector 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:

$$f(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2}\langle \mathbf{k}'|V|\mathbf{k}\rangle = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d\mathbf{r}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} V(\mathbf{r}')$$

which is the Fourier transform of the potential with respect to ***q***, where

$\mathbf{q} = \mathbf{k} - \mathbf{k}'$: scattering wave vector.

For a spherically symmetric potential, $f(\mathbf{k}',\mathbf{k})$ is a function of q.

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

where θ is an angle between ***k***' and ***k*** (Ewald's sphere). Fro simplicity we assume that θ' is an angle between ***q*** and ***r***'. We can perform the angular integration over θ'.

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d\mathbf{r}' e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}')$$
$$= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int_0^\infty dr' \int_0^\pi d\theta' e^{iqr'\cos\theta'} 2\pi r'^2 \sin\theta' V(r')$$

Note that

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

Then

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

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \left| f^{(1)}(\theta) \right|^2$$

18.4 Yukawa potential

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

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

The Yukawa potential is given by

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

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

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

Note that

$$\int_0^\infty dr' e^{-\mu r'} \sin(qr') = \frac{q}{q^2 + \mu^2}$$

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2} \frac{V_0}{\mu} \frac{1}{q^2 + \mu^2}$$

Since

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

so, in the first Born approximation,

$$\frac{d\sigma}{d\Omega} = \left| f^{(1)}(\theta) \right|^2 = \left(\frac{2mV_0}{\mu\hbar^2} \right)^2 \frac{1}{[2k^2(1 - \cos\theta) + \mu^2]^2}$$

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

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

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

Using $E_k = \dfrac{\hbar^2 k^2}{2m}$,

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

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

18.5 Validity of the first-order Born approximation

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

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

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

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

or

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

18.6 Lipmann-Schwinger equation

The Hamiltonian *H* 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

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

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 $(E - \hat{H}_0) |\phi\rangle = 0$, 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

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

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

Lipmann-Schwinger equation:

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

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

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

where

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

and

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

with

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

The Green's function is defined by

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

((**Proof**))

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

or

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

where

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

Then we have

$$I=-\frac{\hbar^2}{2m}\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{\frac{\hbar^2}{2m}(\mathbf{k}^2-\mathbf{k}'^2)\pm i\varepsilon}$$
$$=\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}}{k'^2-(k^2\pm i\varepsilon)}=K_0^{(\pm)}(\mathbf{r}-\mathbf{r}')$$

In summary, we get

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

or

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

More conveniently the Lipmann-Schwinger equation can be rewritten as

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

with

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

and

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

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

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

where $[\hat{A}, \hat{B}] = 0$ are not commutable. 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

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

or

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

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 incoming spherical wave. Note that the operator $\hat{G}^{(\pm)}$ is slightly different from $\hat{G}_0(E_k + i\varepsilon)$,

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

Then we have

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

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

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

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

or

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

18.7 The higher order Born Approximation

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

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

The Lippmann-Schwinger equation is given by

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

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

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

or

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

This is supposed to hold for any $\left|\mathbf{k}\right\rangle$ 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 $f(\mathbf{k}',\mathbf{k})$ can now be written as

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

Using the iteration, we have

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

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

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

with

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

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

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

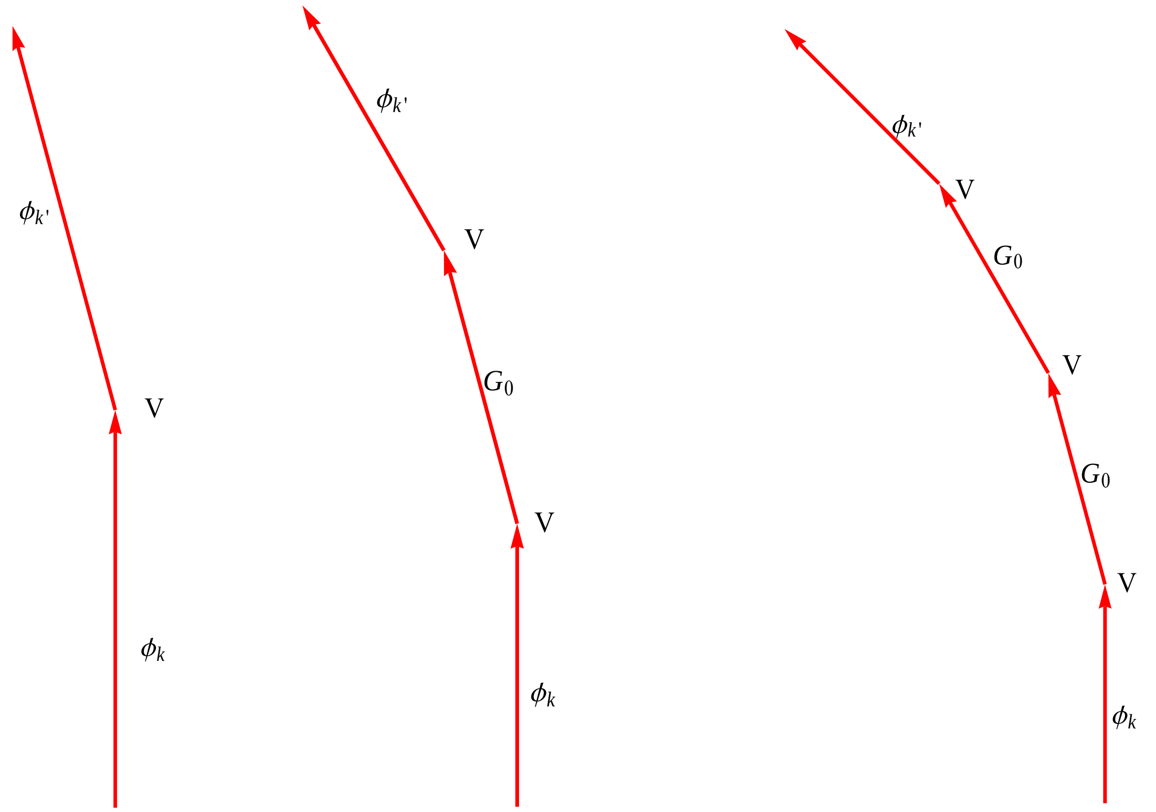


Fig. Feynman diagram. First order, 2nd order, and 3rd order Born approximations. $\phi_k = |\mathbf{k}\rangle$ is the initial state of the incoming particle and $\phi_{k'} = |\mathbf{k}'\rangle$ is the final state of the incoming particle. $\hat{V}$ is the interaction.

18.8 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

$f(\theta = 0) = f(\mathbf{k}, \mathbf{k})$: 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.

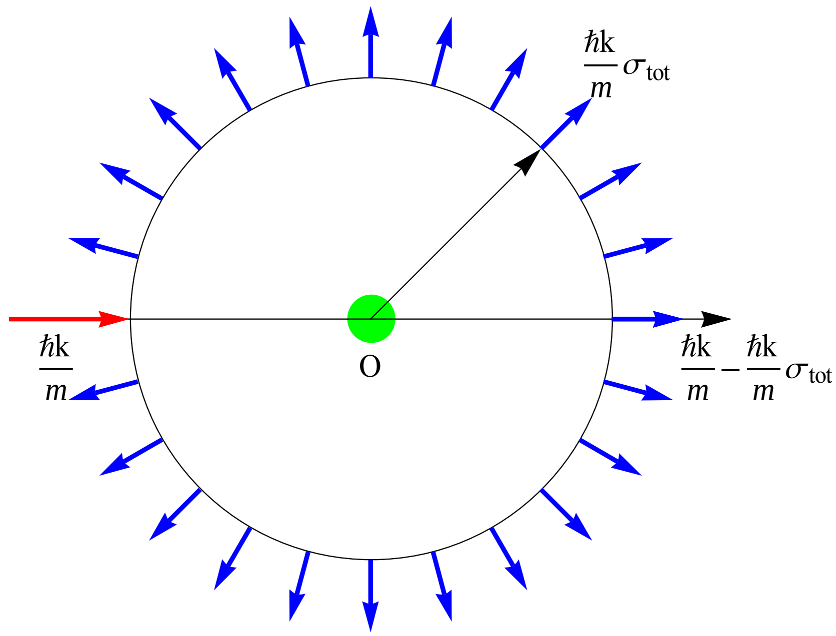


Fig. Optical theorem. The intensity of the incident wave is $\hbar k/m$. The intensity of the forward wave is $(\hbar k/m)-(4\pi\hbar/m)\,\mathrm{Im}[f(0)]$. The waves with the total intensity $(4\pi\hbar/m)\,\mathrm{Im}[f(0)]=(\hbar k/m)\sigma_{tot}$ is scattered for all the directions, as the scattering spherical waves.

((**Proof**))

$$\mathrm{Im}[f(\mathbf{k},\mathbf{k})]=-\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\mathrm{Im}[\langle\mathbf{k}|\hat{T}|\mathbf{k}\rangle]$$
$$=-\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\mathrm{Im}[\langle\mathbf{k}|\hat{V}|\psi^{(+)}\rangle]$$

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

or

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

or

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

Then

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

Now we use the well-known relation

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

Then

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

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

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

Therefore,

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

or

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

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

or

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

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

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

Thus

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

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

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

Since

$$\frac{d\sigma}{d\Omega'} = \left|f(\mathbf{k}',\mathbf{k})\right|^2$$

$$= \frac{1}{16\pi^2}(2\pi)^6 \frac{4m^2}{\hbar^4}\left|\langle \mathbf{k}'|\hat{T}|\mathbf{k}\rangle\right|^2 ,$$

$$= \frac{16\pi^4 m^2}{\hbar^4}\left|\langle \mathbf{k}'|\hat{T}|\mathbf{k}\rangle\right|^2$$

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

Then we obtain

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

REFERENCE

J.J. Sakurai, *Modern Quantum Mechanics*, Revised Edition (Addison-Wesley, Reading Massachusetts, 1994).

A.G. Sitenko and P.J. Shepherd, Lectures in Scattering Theory (Pergamon Press, Oxford, 1971).

E. Merzbacher, Quantum Mechanics 3rd edition (John Wiley & Sons, Inc., New York, 1998).