Note that we did not use $\psi(\vec{r})$ to find the flux but ψ_{in} and ψ_{scatt}. The cross terms were ignored. This is physically reasonable since we ~~have~~ ~~that~~ the incoming wave packet is of finite extent and the scattering detector is considered outside this flux. Also we have reduced the 2 particle scattering to one (relative) particle being scattered from a potential, we are in the C-M frame.

7.1.1. The Scattering Green Function

We can more rigorously determine the above formula and at the same time relate the asymptotic (large r) scattering amplitudes $f(\theta,\phi)$ to the short distance scattering effects of the potential by considering the Green function for the Schrödinger equation with our scattering boundary conditions. The Schrödinger equation is

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

defining $E = \frac{\hbar^2 k^2}{2m} \geq 0$ and $U = \frac{2m}{\hbar^2}V$, this becomes

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

the Helmholtz equation. The Green function $G(\vec{r},\vec{r}\,')$ for the Helmholtz equation is defined as a solution to

$$(\nabla^2 + k^2)G(\vec{r},\vec{r}\,') = \delta^3(\vec{r}-\vec{r}\,').$$

$G(\vec{r},\vec{r}\,')$ is a function of $|\vec{r}-\vec{r}\,'|$ from this. Of course we will have to specify appropriate boundary conditions for G to define it uniquely, as will be done. Proceeding, once we know G the "solution" to the Schrödinger can be obtained as an integral equation

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^{in}(\vec{r}) + \int d^3r'\, G(\vec{r},\vec{r}\,')\,U(\vec{r}\,')\,\psi_{\vec{k}}(\vec{r}\,')$$

where

$$(\nabla^2+k^2)\psi^{in}_{\vec{k}}(\vec{r})=0 \quad \text{is a}$$

solution to the free particle Schrödinger equation, and specifies our incoming particle state, for the plane wave case

$$\psi^{in}_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}.$$

Note $\vec{k}^2=k^2$ is fixed, but the direction is undetermined (infinite degree of degeneracy) and corresponds to choosing the incoming flux direction.

So $\psi_{\vec{k}}(\vec{r})$ obeys the Schrödinger equation since

$$(\nabla^2+k^2)\psi_{\vec{k}}(\vec{r}) = \cancelto{0}{(\nabla^2+k^2)\psi^{in}_{\vec{k}}(\vec{r})}$$

$$+\int d^3r' \underbrace{\left[(\nabla^2+k^2)G(\vec{r},\vec{r}\,')\right]}_{=\delta^3(\vec{r}-\vec{r}\,')} U(\vec{r}\,')\psi_{\vec{k}}(\vec{r}\,')$$

$$=\int d^3r'\, \delta^3(\vec{r}-\vec{r}\,')U(\vec{r}\,')\psi_{\vec{k}}(\vec{r}\,') = U(\vec{r})\psi_{\vec{k}}(\vec{r}).$$

To find G recall that

$$\nabla^2 \frac{1}{|\vec{r}-\vec{r}'|} = -4\pi\delta^3(\vec{r}-\vec{r}') \text{, while}$$

$$\vec{\nabla}\left(e^{\pm ik|\vec{r}-\vec{r}'|}\right) = \pm ik\, e^{\pm ik|\vec{r}-\vec{r}'|}\, \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|}.$$

Thus

$$\nabla^2 e^{\pm ik|\vec{r}-\vec{r}'|} = -k^2 e^{\pm ik|\vec{r}-\vec{r}'|} \pm 2ik\, \frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}.$$

Along with $\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}'|} = -\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^2}$ we find

$$\nabla^2 \frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = \left(\nabla^2 \frac{1}{|\vec{r}-\vec{r}'|}\right) e^{\pm ik|\vec{r}-\vec{r}'|}$$

$$+ \frac{1}{|\vec{r}-\vec{r}'|}\left(\nabla^2 e^{\pm ik|\vec{r}-\vec{r}'|}\right)$$

$$+ 2\left(\vec{\nabla}\frac{1}{|\vec{r}-\vec{r}'|}\right)\cdot\left(\vec{\nabla} e^{\pm ik|\vec{r}-\vec{r}'|}\right)$$

$$= -4\pi\delta^3(\vec{r}-\vec{r}')\, e^{\pm ik|\vec{r}-\vec{r}'|}$$

$$+\left\{-k^2 \cancel{\pm \frac{2ik}{|\vec{r}-\vec{r}\,'|} - 2\frac{(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^2}}\cdot\left(\pm ik\frac{(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\right)\right\}\times$$

$$\times\ \frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$$

$$\Rightarrow\ (\nabla^2+k^2)\,\frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} = -4\pi\,\delta^3(\vec{r}-\vec{r}\,')$$

Thus we have the <u>outgoing</u> G_+ and <u>incoming</u> G_- Green functions

$$G_\pm(\vec{r},\vec{r}\,') \equiv -\frac{1}{4\pi}\,\frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|},$$

and correspondingly the outgoing $\psi_{\vec{k}}^{(+)}$ and incoming $\psi_{\vec{k}}^{(-)}$ solutions to the Schrödinger equation, called the Lippmann-Schwinger equation

$$\psi_{\vec{k}}^{(\pm)}(\vec{r}) = \psi_{\vec{k}}^{in}(\vec{r}) + \int d^3r'\, G_\pm(\vec{r},\vec{r}\,')\,U(\vec{r}\,')\,\psi_{\vec{k}}^{(\pm)}(\vec{r}\,').$$

For large distances $\vec{r}$ with $|\vec{r}| \gg |\vec{r}\,'|$ we have that

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

$$= r - \frac{\vec{r}\cdot\vec{r}'}{r} + O\left(\frac{r'^2}{r^2}\right)$$

Thus
$$G_{\pm}(\vec{r},\vec{r}') \underset{r \gg r'}{\sim} -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}\, e^{\mp ik\frac{\vec{r}\cdot\vec{r}'}{r}}$$

for asymptotic distances r. Hence the the solutions to Schrödinger's equation have the asymptotic form

$$\psi^{(\pm)}_{\vec{k}}(\vec{r}) \sim \psi^{in}_{\vec{k}}(\vec{r}) - \frac{1}{4\pi}\frac{e^{\pm ikr}}{r}\int d^3r'\, e^{\mp ik\frac{\vec{r}\cdot\vec{r}'}{r}} \times$$
$$\times\, U(\vec{r}')\, \psi^{(\pm)}_{\vec{k}}(\vec{r}').$$

Defining the scattered particle's wavevector $\vec{k}' \equiv k\frac{\vec{r}}{r}$ we define the scattering amplitudes

$$\boxed{f^{(\pm)}(\vec{k},\vec{k}') \equiv -\frac{1}{4\pi}\int d^3r'\, e^{\mp\cancel{\pm} i\vec{k}'\cdot\vec{r}'}\, U(\vec{r}')\, \psi^{(\pm)}_{\vec{k}}(\vec{r}')}$$

which are functions of $\vec{k}$ and (θ,φ) independent of r.

Then the asymptotic form of the solution to Schrödinger's equation has the form

$$\psi_{\vec{k}}^{(\pm)}(\vec{r}) \sim \psi_{\vec{k}}^{in}(\vec{r}) + f^{(\pm)}(\vec{k},\vec{k}') \frac{e^{\pm ikr}}{r} .$$

We have that the time dependence of the stationary state is simply $e^{-\frac{i}{\hbar}Et}$; thus

$$\psi_{\vec{k}}^{(\pm)}(\vec{r},t) \sim \psi_{\vec{k}}^{in}(\vec{r},t) + \frac{f^{(\pm)}(\vec{k},\vec{k}')}{r} e^{-\frac{i}{\hbar}(Et \mp ikr)}$$

Hence $\psi_{\vec{k}}^{(+)}$ contains an outgoing scattered spherical wave while $\psi_{\vec{k}}^{(-)}$ contains an incoming scattered spherical wave. Correspondingly $G_{\pm}(\vec{r},\vec{r}')$ are the outgoing $(+)$ and incoming $(-)$ scattering Green functions. Since we are interested in particles scattered out to our detector from the scattering center that G_+ and $\psi^{(+)}_{\vec{k}}$ have the correct boundary conditions for that case. Thus we find

$$\psi^{(+)}_{\vec{k}}(\vec{r}) \sim \psi^{in}_{\vec{k}}(\vec{r}) + f^{(+)}(\vec{k},\vec{k}')\,\frac{e^{+ikr}}{r}$$

and, as earlier, the differential cross section is given as

$$\sigma(\theta,\varphi) = |f^{(+)}(\vec{k},\vec{k}')|^2 .$$

The scattering amplitudes $f^{(+)}(\vec{k},\vec{k}')$ are given by

$$f^{(+)}(\vec{k},\vec{k}') = -\frac{1}{4\pi}\int d^3r'\, e^{-i\vec{k}'\cdot\vec{r}'}\, U(\vec{r}')\,\psi^{(+)}_{\vec{k}}(\vec{r}')$$
$$\equiv f(\theta,\varphi) .$$

To determine $f(\theta,\varphi)$ we must find the solution to the Schrödinger equation $\psi^{(+)}_{\vec{k}}(\vec{r})$ in the region where the potential $V(\vec{r})$ is non-zero. That is we must solve the integral equation

$$= -\frac{1}{4\pi}\frac{e^{+ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

$$\psi^{(+)}_{\vec{k}}(\vec{r}) = \underbrace{\psi^{in}_{\vec{k}}(\vec{r})}_{=e^{i\vec{k}\cdot\vec{r}}} + \underbrace{\int d^3r'\,\overbrace{G_+(\vec{r},\vec{r}')}\,U(\vec{r}')\,\psi^{(+)}_{\vec{k}}(\vec{r}')}_{\equiv \psi_{scattered}(\vec{r})}$$

Of course we will not be able to solve this integral equation exactly and must resort to approximation techniques.

First, let's consider the determination of the Green function by solving the Helmholtz equation by Fourier transform. That is

$$G(\vec{r},\vec{r}') \equiv \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\,\tilde{G}(\vec{q})$$

So that the Green function equation

$$(\nabla^2 + k^2)\,G(\vec{r},\vec{r}') = \delta^3(\vec{r}-\vec{r}')$$

becomes

$$(-\vec{q}^{\,2} + k^2)\,\tilde{G}(\vec{q}) = 1$$

$$\Rightarrow \quad \tilde{G}(\vec{q}) = \frac{-1}{\vec{q}^{\,2} - k^2} \quad \text{away from } \vec{q}^{\,2} = k^2.$$

It still remains to define $\tilde{G}(\vec{q})$ for $\vec{q}^{\,2} = k^2$. As will be seen, this is equivalent to specifying the coordinate space boundary conditions. Corresponding to the incoming and outgoing spherical wave boundary conditions we replace k by $k \pm i\epsilon$ where $\epsilon > 0$ is a small positive number which we take to zero after the various integrals are performed. Thus we have two Fourier coefficients

$$\tilde{G}_\pm(\vec{q}) = \frac{-1}{\vec{q}^{\,2} - (k \pm i\epsilon)^2}$$

$$\left(\tilde{G}_\pm(\vec{q}) = \frac{-1}{\vec{q}^{\,2} - k^2 \mp 2i\epsilon [illegible]} = \frac{1}{k^2 - \vec{q}^{\,2} [illegible]} \right)$$

which as we shall see directly, give the outgoing and incoming scattering Green functions, $G_\pm(\vec{r}, \vec{r}\,')$.

So
$$G_\pm(\vec{r}, \vec{r}\,') = \lim_{\epsilon \to 0^+} \int \frac{d^3q}{(2\pi)^3} \frac{-e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}}{\vec{q}^{\,2} - (k \pm i\epsilon)^2}$$

Using spherical polar coordinates for $\vec{q}$ we have, with the limit $\epsilon \to 0^+$ understood at the end,

$$G_{\pm}(\vec{r},\vec{r}\,') = -\frac{1}{8\pi^3}\int_0^\infty dq \frac{q^2}{q^2-(k\pm i\epsilon)^2} \times$$

$$\times \int_0^{2\pi} d\varphi \int_{-1}^{+1} d(\cos\theta)\, e^{iq|\vec{r}-\vec{r}\,'|\cos\theta}$$

$$= -\frac{1}{4\pi^2}\int_0^\infty dq \frac{q^2}{q^2-(k\pm i\epsilon)^2} \times$$

$$\times \frac{1}{iq|\vec{r}-\vec{r}\,'|}\left(e^{iq|\vec{r}-\vec{r}\,'|} - e^{-iq|\vec{r}-\vec{r}\,'|}\right)$$

$$= \frac{-1}{4\pi^2 i|\vec{r}-\vec{r}\,'|}\left[\int_0^\infty dq \frac{q e^{iq|\vec{r}-\vec{r}\,'|}}{q^2-(k\pm i\epsilon)^2}\right.$$

$$\left. \underbrace{-\int_0^\infty dq \frac{q e^{-iq|\vec{r}-\vec{r}\,'|}}{q^2-(k\pm i\epsilon)^2}}\right]$$

let $q \to -q$ in the second term

$$= +\int_{-\infty}^0 dq \frac{q e^{+iq|\vec{r}-\vec{r}\,'|}}{q^2-(k\pm i\epsilon)^2}$$

Thus

$$G_{\pm}(\vec{r},\vec{r}') = \frac{-1}{2\pi|\vec{r}-\vec{r}'|}\int_{-\infty}^{+\infty}\frac{dq}{2\pi i}\,\frac{q\,e^{+iq|\vec{r}-\vec{r}'|}}{q^2-(k\pm i\epsilon)^2}$$

As suggested by the form of the integral, we can evaluate it by the methods of contour integration. The integrand has simple poles given by

$$0 = q^2-(k\pm i\epsilon)^2$$
$$= [q+(k\pm i\epsilon)][q-(k\pm i\epsilon)] .$$

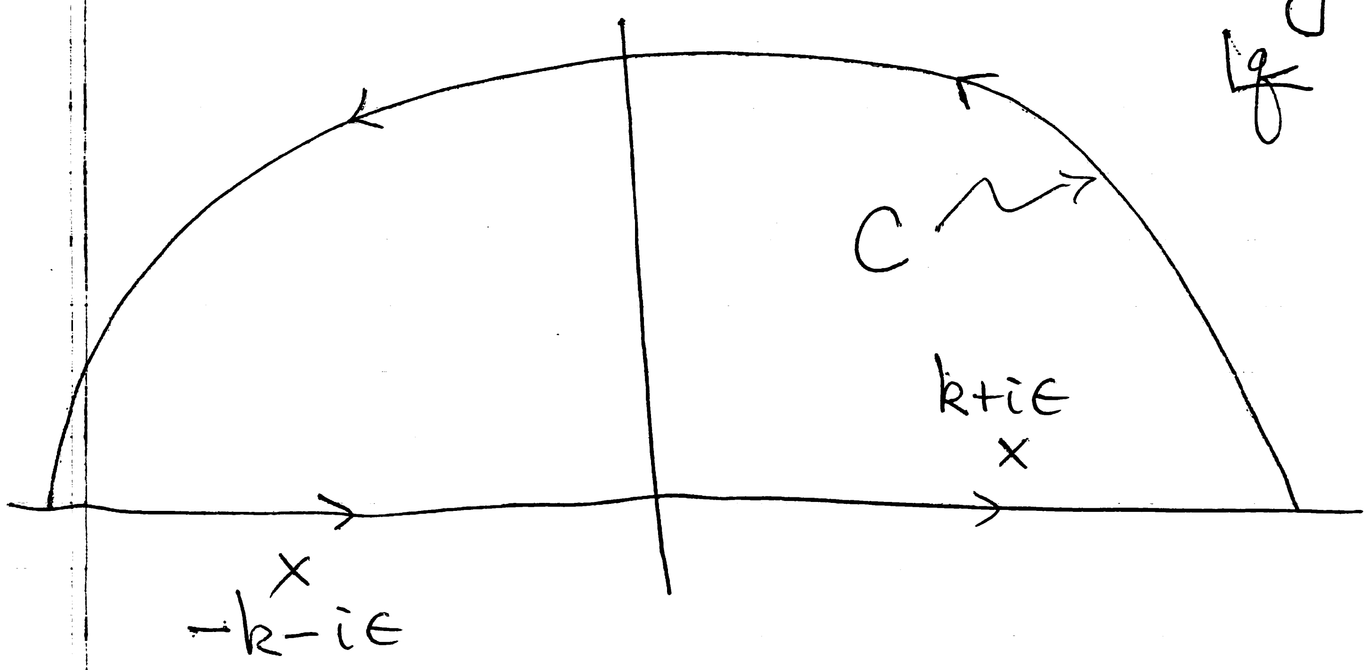
Thus $\tilde{G}_{\pm}(\vec{q})$ has simple poles at

$$q = k\pm i\epsilon \quad \text{and} \quad q = -k\mp i\epsilon .$$

Consider G_+ first, $\tilde{G}_+(\vec{q})$ has the simple poles at $q = k+i\epsilon$ and $q=-k-i\epsilon$. Extending q to the complex plane, we note that for q in the upper half plane, i.e. $q = q_R + iq_I$, $q_I > 0$, The exponential becomes

$$e^{+iq|\vec{r}-\vec{r}'|} = e^{iq_R|\vec{r}-\vec{r}'|}\, e^{-q_I|\vec{r}-\vec{r}'|}$$

providing an exponential damping of the integrand. Hence, we can close the real axis contour in the upper half plane since the integrand vanishes on the semi-circle at infinity



Thus

$$G_+(\vec{r},\vec{r}') = \frac{-1}{2\pi|\vec{r}-\vec{r}'|} \oint_C \frac{dq}{2\pi i} \frac{q\, e^{+iq|\vec{r}-\vec{r}'|}}{[q-(k+i\epsilon)][q+(k+i\epsilon)]}$$

C encloses the simple pole at $q = k+i\epsilon$ only, hence by Cauchy's residue theorem we find

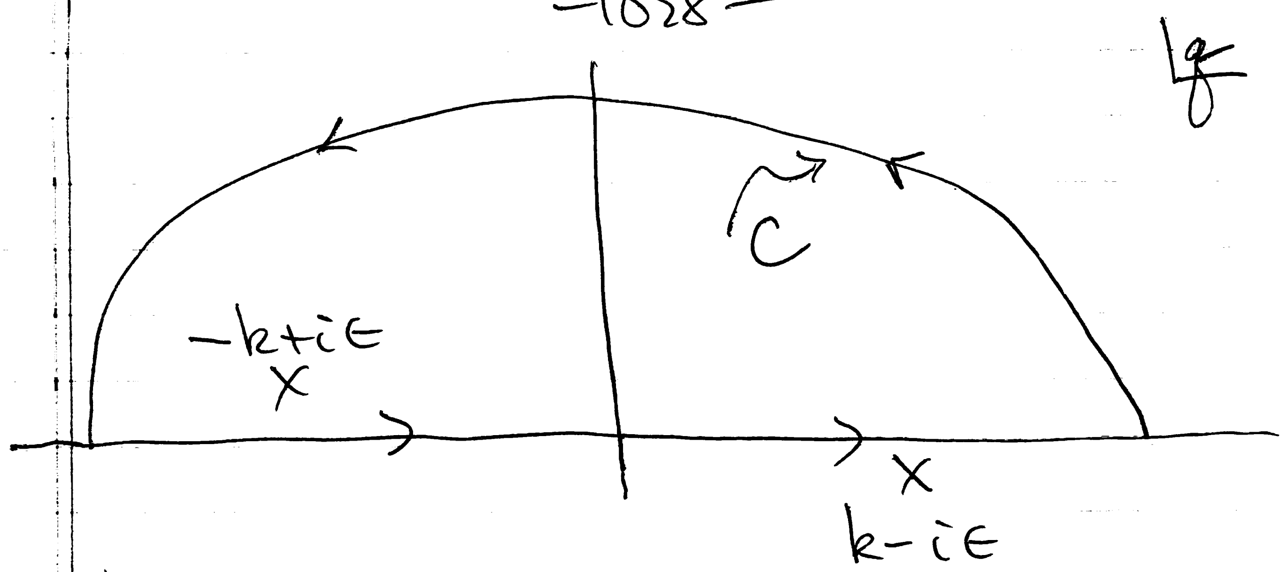
$$G_+(\vec{r},\vec{r}\,') = \frac{-1}{2\pi|\vec{r}-\vec{r}\,'|} \frac{(k+i\epsilon)e^{+i(k+i\epsilon)|\vec{r}-\vec{r}\,'|}}{2(k+i\epsilon)}$$

which in the $\epsilon \to 0^+$ limit is finite and

$$\boxed{G_+(\vec{r},\vec{r}\,') = -\frac{e^{+ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|}}$$

our previous result on page -1018-.

Similarly for G_-, the integrand is analytic everywhere in the upper half plane except at the simple pole $q = -k + i\epsilon$. As before $e^{+iq|\vec{r}-\vec{r}\,'|}$ damps the integrand in the upper half complex q-plane so we can close the contour above the real axis as previously with a semi-circle at infinity



Hence

$$G_-(\vec{r},\vec{r}') = \frac{-1}{2\pi|\vec{r}-\vec{r}'|}\oint_C \frac{dq}{2\pi i}\,\frac{q\,e^{+iq|\vec{r}-\vec{r}'|}}{[q+(k-i\epsilon)][q-(k-i\epsilon)]}$$

Performing the integral by residues

$$G_-(\vec{r},\vec{r}') = \frac{-1}{2\pi|\vec{r}-\vec{r}'|}\,\frac{(-k+i\epsilon)\,e^{i(-k+i\epsilon)|\vec{r}-\vec{r}'|}}{2(-k+i\epsilon)}$$

Taking the well defined $\epsilon \to 0^+$ limit we obtain

$$\boxed{G_-(\vec{r},\vec{r}') = \frac{-1}{4\pi}\,\frac{e^{-ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}}$$

again in agreement

with our previous result on page -1018-.