7.2. Scattering by a Central Potential and the Partial Wave Analysis

In the case that the potential is central the stationary state wavefunction factorize into a radial solution times the spherical harmonics, the eigenfunction of $\vec{L}^2$ and L_z

$$\psi^{(+)}_{k,l,m}(\vec{r}) = R_{kl}(r)\, Y_l^m(\theta,\varphi)$$

where the Schrödinger equation reduces to just the radial equation for R_{kl}

$$R_{kl} \equiv \frac{1}{r}\, u_{kl}(r)$$

with

$$\left(\frac{d^2}{dr^2}+k^2\right)u_{kl}(r) = \left[\frac{l(l+1)}{r^2} + U(r)\right]u_{kl}(r).$$

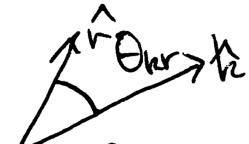
and $u_{kl}(r=0)=0$. Rather than work with the differential equation and boundary condition we can combine the two into the Lippmann–Schwinger integral equation as before. That is we can expand $\psi^{(+)}(\vec{r})$ in terms of spherical harmonics. Along with it we also must expand $G_+(\vec{r},\vec{r}')$

and $e^{i\vec{k}\cdot\vec{r}}$ in terms of spherical harmonics. (Gottfried: section 14.)

The plane wave solution we already have expanded (pages -721- to -735-) to find

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l \, Y_l^{m*}(\theta_{\vec{k}}, \varphi_{\vec{k}}) \, j_l(kr) \, Y_l^m(\theta, \varphi).$$

[Recall this result followed from the expansion of $e^{i\vec{k}\cdot\vec{r}}$ as

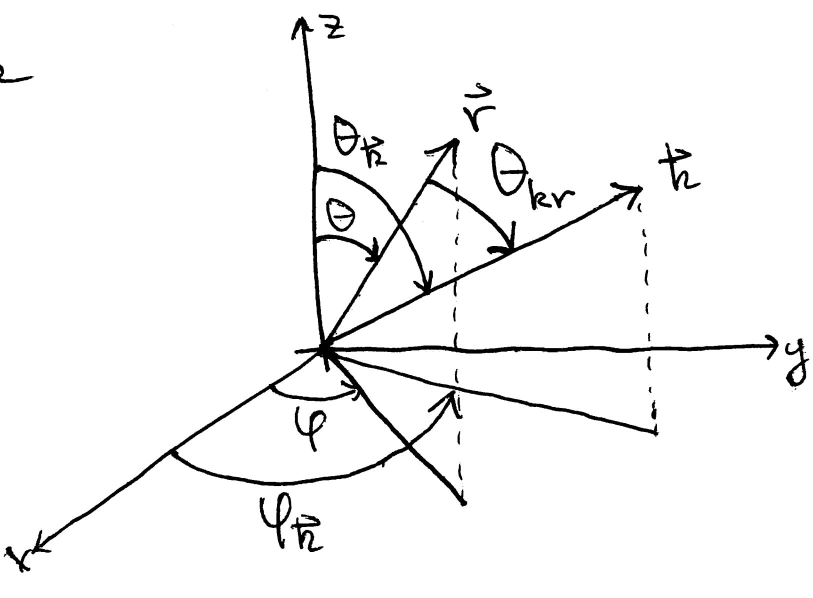


$$e^{i\vec{k}\cdot\vec{r}} = \sum_{l=0}^{\infty} i^l (2l+1) \, j_l(kr) \, P_l(\hat{k}\cdot\hat{r}) \,, \quad \text{(Bauer formula)}$$

and the use of the addition theorem for spherical harmonics

$$P_l(\hat{k}\cdot\hat{r}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y_l^{m*}(\theta_{\vec{k}}, \varphi_{\vec{k}}) \, Y_l^m(\theta, \varphi)$$

where



.)

The Green function $G_+(|\vec{r}-\vec{r}'|)$ has the expansion

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

$$= -ik\sum_{l=0}^{\infty}\frac{(2l+1)}{4\pi}\, j_l(kr_<)\,h_l(kr_>)\,P_l(\hat{r}\cdot\hat{r}')$$

$$= -ik\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} j_l(kr_<)\,h_l(kr_>)\,Y_l^{m*}(\theta',\varphi')\times$$
$$\times Y_l^{m}(\theta,\varphi)$$

where $h_l(\rho) = h_l^{(1)}(\rho) = j_l(\rho) + i n_l(\rho)$ is the spherical Hankel function (Schiff p.86-87) (note $h_l^{(2)} \equiv j_l - i n_l = h_l^{*}$) and j_l is the spherical Bessel function, while n_l the spherical Neumann function (Schiff p.85-86) and $r_>$ is the greater of (r,r') while $r_<$ is the lesser of (r,r').

i.e. $r_> = \begin{cases} r & \text{if } r > r' \\ r' & \text{if } r' > r \end{cases}$ (Butkov Chap. 14 prob. 5, 6)

$$r_< = \begin{cases} r & \text{if } r < r' \\ r' & \text{if } r' < r \end{cases}.$$

To derive this equation, note that all the angular dependence in

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

comes from $\hat{r}\cdot\hat{r}'$ in

$$|\vec{r}-\vec{r}\,'| = \left(r^2+r'^2-2rr'\hat{r}\cdot\hat{r}'\right)^{1/2}.$$

Thus expanding $G_+(\vec{r},\vec{r}\,')$ in terms of $P_\ell(\hat{r}\cdot\hat{r}')$, we have

$$G_+(\vec{r},\vec{r}\,') = \sum_{\ell=0}^{\infty}(2\ell+1)\,G_+^\ell(r,r')\,P_\ell(\hat{r}\cdot\hat{r}')$$

$$= 4\pi\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} G_+^\ell(r,r')\,Y_\ell^{m*}(\theta',\varphi')\,Y_\ell^m(\theta,\varphi).$$

Now to find $G_+^\ell(r,r')$ we must perform

The angular integrals in the Fourier transform representation of G_+

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

$$= -\int d\Omega_{\vec{q}} \int_0^\infty \frac{dq\, q^2}{(2\pi)^3} \frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}}{q^2-(k+i\epsilon)^2}$$

Using the expansion of a plane wave in terms of spherical harmonics, we find

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

$$\times \underbrace{\left[4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(qr) Y_l^{m*}(\theta_{\vec{q}},\varphi_{\vec{q}}) Y_l^m(\theta,\varphi)\right]}_{=e^{i\vec{q}\cdot\vec{r}}}$$

$$\times \underbrace{\left[4\pi \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} i^{l'} j_{l'}(qr') Y_{l'}^{m'*}(\theta_{\vec{q}},\varphi_{\vec{q}}) Y_{l'}^{m'}(\theta',\varphi')\right]^*}_{=e^{-i\vec{q}\cdot\vec{r}\,'} = \left(e^{+i\vec{q}\cdot\vec{r}\,'}\right)^*}$$

$$= -\frac{2}{\pi}\sum_{l'=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m'=-l'}^{+l'}\sum_{m=-l}^{+l} i^{l}(-i)^{l'} Y_{l'}^{m'}(\theta',\varphi') Y_{l}^{m}(\theta,\varphi)^{*}$$

$$\times \int_0^\infty dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_l(qr) j_{l'}(qr') \times$$

$$\times \underbrace{\int d\Omega_{\vec{q}}\, Y_l^{m*}(\theta_{\vec{q}},\varphi_{\vec{q}}) Y_{l'}^{m'}(\theta_{\vec{q}},\varphi_{\vec{q}})}_{=\delta_{ll'}\delta_{mm'}}$$

$$\boxed{G_+(\vec{r},\vec{r}') = 4\pi \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y_l^{m*}(\theta',\varphi') Y_l^{m}(\theta,\varphi) \times \left[\frac{-1}{2\pi^2}\int_0^\infty dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_l(qr) j_l(qr')\right]}$$

Comparing this with the expansion on the previous page -1051- we have that the coefficients $G_+^l(r,r')$ are

$$\boxed{G_+^l(r,r') = -\frac{1}{2\pi^2}\int_0^\infty dq\, \frac{q^2}{q^2-(k+i\epsilon)^2}\, j_l(qr)\, j_l(qr')}$$

Since $j_l(-\rho) = (-1)^l j_l(\rho)$, the integrand above is even and we can extend the integration over the whole real line by dividing by 2

$$G_+^l(r,r') = -\frac{1}{4\pi^2}\int_{-\infty}^{+\infty} dq\, \frac{q^2}{q^2-(k+i\epsilon)^2}\, j_l(qr)\, j_l(qr').$$

As usual, we can perform this integral by the method of contours. To do that we exploit the properties of j_l, h_l, n_l;

$$j_l(\rho) = \frac{1}{2}\left[h_l(\rho) + h_l^*(\rho)\right]$$

where

$$h_l(\rho) \underset{\rho\to\infty}{\sim} \frac{1}{\rho}\, e^{i(\rho-(l+1)\frac{\pi}{2})}$$

$$h_l^*(\rho) \underset{\rho\to\infty}{\sim} \frac{1}{\rho}\, e^{-i(\rho-(l+1)\frac{\pi}{2})}$$

and

$$j_\ell(\rho) \underset{\rho\to\infty}{\sim} \frac{1}{2\rho}\left[e^{i(\rho-(\ell+1)\frac{\pi}{2})} + e^{-i(\rho-(\ell+1)\frac{\pi}{2})}\right].$$

First for $\underline{r > r'}$, we have

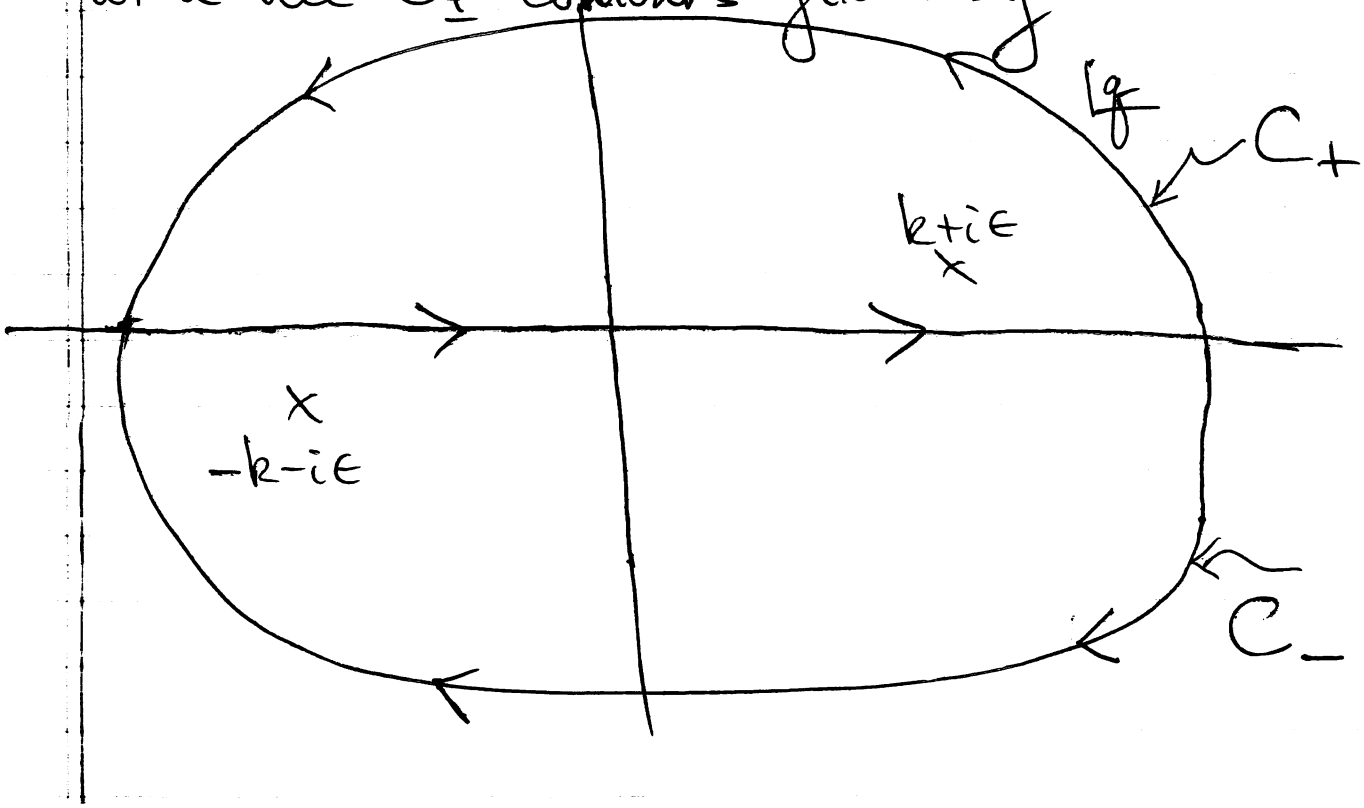
$$G_+^\ell(r,r') = -\frac{1}{8\pi^2}\int_{-\infty}^{+\infty} dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_\ell(qr') \times$$

$$\times \left[h_\ell(qr) + h_\ell^*(qr)\right] \Big|_{r>r'}.$$

Recall that $j_\ell(qr)$ is an entire function of q while $h_\ell(qr)$ and $h_\ell^*(qr)$ have simple poles at $q=0$. But the integrand is well behaved at $q=0$ due to the q^2 factor in the numerator. Hence the only singularities of the integrand are the simple poles at $q = \pm(k+i\epsilon)$. Since $r>r'$, the integral over the real axis can be closed to include a semi-circle at infinity. For the $(h_\ell^*(qr))$ $h_\ell(qr)$ term, the semi-circle is in the (lower) upper half plane where the integrand exponentially goes to zero. That is for $r>r'$, $(h_\ell^*(qr))$ $h_\ell(qr)$ exponentially vanishes at a rate faster than $j_\ell(qr')$ exponentially grows as $|q|\to\infty$ on the semi-circle in the ~~(lower)~~ upper half-plane. Thus the Green function becomes

$$G_+^\ell(r,r') = -\frac{1}{8\pi^2}\left[\oint_{C_+} dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_\ell(qr')h_\ell(qr) + \oint_{C_-} dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_\ell(qr')h_\ell^*(qr)\right]\Bigg|_{r>r'}$$

with the $C_\pm$ contours given by



Thus C_+ encloses the simple pole at $q = k + i\epsilon$ while C_- encloses the simple pole at $q = -(k+i\epsilon)$. Using the Residue (Cauchy) theorem we find, taking the now innocuous $\epsilon \to 0^+$, (recall $q^2 - (k+i\epsilon)^2 = [q-(k+i\epsilon)][q+(k+i\epsilon)]$)

$$G_+^l(r,r') = -\frac{1}{8\pi^2}(2\pi i)\left[\frac{k^2}{2k} j_l(kr')h_l(kr)\right.$$

(since C_- is clockwise)

$$\left. - \frac{(-k)^2}{2(-k)} j_l(-kr')h_l^*(-kr)\right]\Bigg|_{r>r'}$$

$$= \frac{-ik}{8\pi}\left[j_l(kr')h_l(kr) + j_l(-kr')h_l^*(-kr)\right]\Bigg|_{r>r'}$$

Now $j_l(-\rho) = (-1)^l j_l(\rho)$ and $h_l^*(-\rho) = (-1)^l h_l(\rho)$ so that $j_l(-\rho)h_l^*(-\rho) = j_l(\rho)h_l(\rho)$. Hence

$$\boxed{G_+^l(r,r') = \frac{-ik}{4\pi} j_l(kr')h_l(kr) \quad \text{for } r > r'}$$

Next consider $r<r'$. Proceeding as before with $j_\ell(qr') = h_\ell(qr') + h_\ell^*(qr')$ ~~need~~ damping ~~the~~ integrand on $C_\pm$. Thus we ~~have~~

$$G_+^\ell(r,r') = -\frac{1}{8\pi^2}\left[\oint_{C_+} dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_\ell(qr)\,h_\ell(qr') + \oint_{C_-} dq \frac{q^2}{q^2-(k+i\epsilon)^2} j_\ell(qr)\,h_\ell^*(qr')\right]_{r<r'}$$

Thus we find for $r<r'$

$$\boxed{G_+^\ell(r,r') = \frac{-ik}{4\pi} j_\ell(kr)\,h_\ell(kr')}$$

Combining these two cases, we have that

$$\boxed{G_+^\ell(r,r') = -\frac{ik}{4\pi} j_\ell(kr_<)\,h_\ell(kr_>)}$$

Substituting this into G_+ on page -1051- we find the result originally claimed on page -1050-

$$\boxed{\begin{aligned} G_+(\vec{r},\vec{r}') &= -\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \\ &= -ik\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} j_l(kr_<)h_l(kr_>)Y_l^{m*}(\theta',\varphi')Y_l^m(\theta,\varphi) \end{aligned}}$$

We can now turn to the Lippmann-Schwinger equation for the scattering wavefunction

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int d^3r'\, G_+(\vec{r},\vec{r}')U(r')\psi_{\vec{k}}^{(+)}(\vec{r}')$$

central potential $U(\vec{r}') = U(r')$

Since $\psi_{\vec{k}}^{(+)}(\vec{r})$ is a scalar function under rotations it can only be a function of $\vec{r}^2$, $\vec{k}^2$ and $\vec{k}\cdot\vec{r}$, that is the only angular dependence is from $\hat{k}\cdot\hat{r}$. Thus we can expand $\psi_{\vec{k}}^{(+)}(\vec{r})$ in terms of $P_l(\hat{k}\cdot\hat{r})$ and then use the addition theorem for spherical harmonics

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = \sum_{l=0}^{\infty} (2l+1) i^l \psi_l^{(+)}(r) P_l(\hat{k}\cdot\hat{r})$$

$$= 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l \psi_l^{(+)}(r) Y_l^{m*}(\theta_k, \varphi_k) Y_l^m(\theta,\varphi)$$

Now we substitute our expansion for the plane wave and $G_+(\vec{r},\vec{r}\,')$

(Note $e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_l^{m*}(\theta_k,\varphi_k) Y_l^m(\theta,\varphi)$

$\Rightarrow \psi_l^{(+)}(r) = j_l(kr)$ for plane waves i.e. $U(r) = 0$.)

So

$\psi_{\vec{k}}^{(+)}(\vec{r}) - e^{i\vec{k}\cdot\vec{r}}$

$$= 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l \left[\psi_l^{(+)}(r) - j_l(kr)\right] Y_l^{m*}(\theta_k,\varphi_k) Y_l^m(\theta,\varphi)$$

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

$$= \int d\Omega'_{\vec{r}'} \int_0^\infty dr'\, r'^2\, U(r') \times$$

$$\times \underbrace{\left[4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} G_+^l(r,r')\, Y_l^m(\theta,\varphi)\, Y_l^{m*}(\theta',\varphi') \right]}_{= G_+(\vec{r},\vec{r}')} \times$$

$$\times \underbrace{\left[4\pi \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} i^{l'}\, \psi_{l'}^{(+)}(r')\, Y_{l'}^{m'}(\theta',\varphi')\, Y_{l'}^{m'*}(\theta_{\vec{k}},\varphi_{\vec{k}}) \right]}_{= \psi_{\vec{k}}^{(+)}(\vec{r}')}$$

$$= (4\pi)^2 \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} i^{l'}\, Y_l^m(\theta,\varphi)\, Y_{l'}^{m'*}(\theta_{\vec{k}},\varphi_{\vec{k}}) \times$$

$$\times \int_0^\infty dr'\, r'^2\, U(r')\, G_+^l(r,r')\, \psi_{l'}^{(+)}(r') \times$$

$$\times \underbrace{\int d\Omega'_{\vec{r}'}\, Y_l^{m*}(\theta',\varphi')\, Y_{l'}^{m'}(\theta',\varphi')}_{= \delta_{ll'}\,\delta_{mm'}}$$

Thus

$$4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l \left[\mathcal{U}_l^{(+)}(r) - j_l(kr) \right] Y_l^{m*}(\theta_k, \varphi_k) Y_l^m(\theta, \varphi)$$

$$= 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l \left[4\pi \int_0^{\infty} dr' \, r'^2 \, U(r') G_+^l(r, r') \mathcal{U}_l^{(+)}(r') \right] \times$$

$$\times Y_l^{m*}(\theta_k, \varphi_k) Y_l^m(\theta, \varphi)$$

Since $Y_l^m(\theta, \varphi)$ and $Y_l^{m*}(\theta_k, \varphi_k)$ are linearly independent, each term above must be equal $\Rightarrow$

$$\boxed{\mathcal{U}_l^{(+)}(r) = j_l(kr) + 4\pi \int_0^{\infty} dr' \, r'^2 \, G_+^l(r, r') U(r') \times \mathcal{U}_l^{(+)}(r')} \; .$$

The central potential implies that the radial wavefunctions for each l decouple. The $\mathcal{U}_l^{(+)}(r)$ is called the <u>l^{th} partial wave</u>. Hence, as expected from the Schrödinger differential equation the scattering from a central potential is reduced to an effective one-dimensional radial Lippmann-Schwinger integral equation.

Recall that the scattering amplitude and cross-section are given by the asymptotic behavior as $r \to \infty$ of $\psi^{(+)}_{\vec{k}}(\vec{r})$. Since

$$h_\ell(kr) \underset{r\to\infty}{\sim} \frac{1}{kr} e^{i[kr-(\ell+1)\frac{\pi}{2}]}$$

we have

$$G^\ell_+(r,r') = \frac{-ik}{4\pi} j_\ell(kr') h_\ell(kr)$$

$$\underset{r\to\infty}{\sim} \frac{-ik}{4\pi} j_\ell(kr') \frac{1}{kr} e^{i[kr-(\ell+1)\frac{\pi}{2}]}$$

implying that

$$\psi^{(+)}_\ell(r) \underset{r\to\infty}{\sim} j_\ell(kr) + \frac{e^{ikr}}{r}\Big[-i e^{-i(\ell+1)\frac{\pi}{2}} \times$$

$$\times \int_0^\infty dr' r'^2 U(r') j_\ell(kr') \psi^{(+)}_\ell(r')\Big]$$

Now $e^{-i(\ell+1)\frac{\pi}{2}} = (-i)^{\ell+1}$ we find

$$\boxed{\psi_\ell^{(+)}(r) \underset{r\to\infty}{\sim} j_\ell(kr) + \frac{e^{ikr}}{r}\left[(-i)^{\ell+2}\int_0^\infty dr'\, r'^2 \times U(r')\, j_\ell(kr')\, \psi_\ell^{(+)}(r')\right].}$$

Multiplying by $(2\ell+1)i^\ell P_\ell(\hat{k}\cdot\hat{r})$ and summing over all ℓ, using

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell\,\psi_\ell^{(+)}(r)\,P_\ell(\hat{k}\cdot\hat{r})$$

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell\, j_\ell(kr)\,P_\ell(\hat{k}\cdot\hat{r}),$$

we have

$$\psi_{\vec{k}}^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r} f^{(+)}(\vec{k},\vec{k}')$$

with

$$f^{(+)}(\vec{k},\vec{k}') = -\sum_{l=0}^{\infty}(2l+1)P_l(\hat{k}\cdot\hat{r}) \times$$

$$\times \int_0^\infty dr' r'^2 U(r') j_l(kr') \psi_l^{(+)}(r'),$$

the exact scattering amplitude.

Recall that $\vec{k}' = k\hat{r}$, so defining

$$\boxed{S_l(k) \equiv 1 - 2ik\int_0^\infty dr' r'^2 j_l(kr') U(r') \psi_l^{(+)}(r')}$$

we have

$$\boxed{f^{(+)}(\vec{k},\vec{k}') = \sum_{l=0}^{\infty}(2l+1)\left[\frac{S_l(k)-1}{2ik}\right]P_l(\hat{k}\cdot\hat{k}')}\ .$$

As usual to find the exact $S_l(k)$, and so $f^{(+)}(\vec{k},\vec{k}')$, we must solve the integral equation for $\psi_l^{(+)}(r)$.

With $S_l(k)$ so defined the asymptotic form of the l^{th} partial wave becomes

$$\psi_l^{(+)}(r) \underset{r\to\infty}{\sim} j_l(kr) - i\,\frac{e^{i[kr-(l+1)\frac{\pi}{2}]}}{r}\left[\frac{S_l(k)-1}{-2ik}\right],$$

using $j_l(kr) \underset{r\to\infty}{\sim} \frac{1}{2kr}\left(e^{i[kr-(l+1)\frac{\pi}{2}]} + e^{-i[kr-(l+1)\frac{\pi}{2}]}\right)$

we have

$$\boxed{\psi_l^{(+)}(r) \underset{r\to\infty}{\sim} \frac{1}{2kr}\left(S_l(k)\,e^{i[kr-(l+1)\frac{\pi}{2}]} + e^{-i[kr-(l+1)\frac{\pi}{2}]}\right)}$$

If $U=0$ so there is no scattering, then $S_l(k)=1$ and $\psi_l^{(+)}(r) \underset{r\to\infty}{\sim} j_l(kr)$ that is $\psi_{\vec{k}}^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} e^{i\vec{k}\cdot\vec{r}}$. The wavefunction remains the plane wave; it is the only outgoing (as well as incoming) wave.

Thus we see that when there is ($U\neq 0$) scattering $S_l(k)\neq 1$ and the coefficient of the outgoing spherical wave is changed.

from its plane wave value. All the effects of scattering are simply contained in the numbers $S_\ell(k)$.

For potential scattering from a real potential $S_\ell(k)$ is just a phase,

$$|S_\ell(k)|=1 \Rightarrow S_\ell(k)=e^{2i\delta_\ell(k)} \text{ with}$$

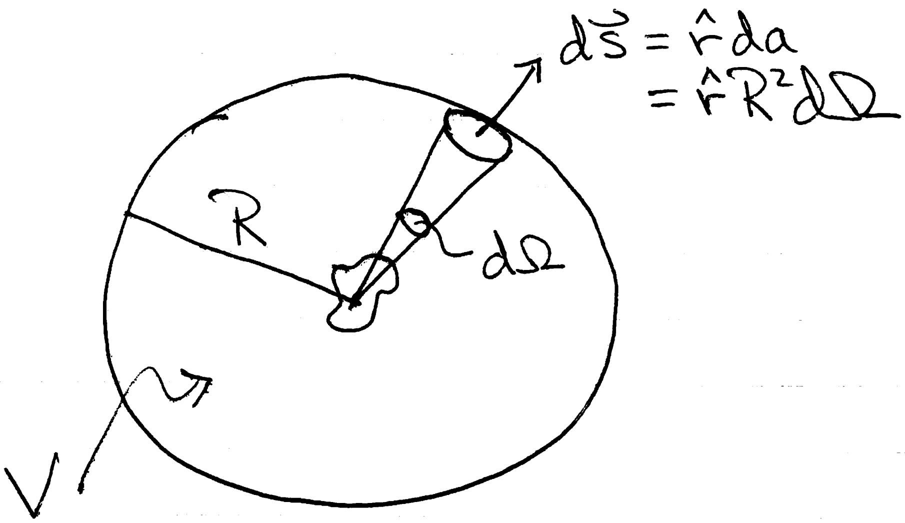
$\delta_\ell \in \mathbb{R}$. $\delta_\ell(k)$ is called the <u>phase shift</u>.

Then asymptotically

$$\psi_\ell^{(+)}(r) \underset{r\to\infty}{\sim} \frac{1}{2kr}\left(e^{i[kr-(\ell+1)\frac{\pi}{2}+2\delta_\ell]} + e^{-i[kr-(\ell+1)\frac{\pi}{2}]}\right).$$

The total effects of scattering are simply to change the phase of the outgoing spherical wave.

To show that $|S_\ell(k)|=1$ we exploit the conservation of probability. Consider a sphere of radius R surrounding the scattering center and enclosing a volume V.



$\rho = \psi_k^{(+)}(\vec{r})^* \psi_k^{(+)}(\vec{r})$ is the probability density. Since U is <u>real</u>, ρ is time independent and we have directly

$$\frac{d}{dt}\int_V d^3r\,\rho = \int_V d^3r\,\frac{\partial\rho}{\partial t} = 0 .$$

The continuity equation $\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0$ then yields

$$0 = \int_V \frac{\partial\rho}{\partial t}\,d^3r = -\int_V d^3r\,\vec{\nabla}\cdot\vec{J} = -\oint_S \vec{J}\cdot d\vec{S}$$

So

$$\oint_S \vec{J}\cdot\hat{r}\,da = 0 ,$$

no net probability flux flows in or out of the volume.

Recalling that the probability current is

$$\vec{J} = \frac{\hbar}{2im}\left[\psi_{\vec{k}}^{(+)*}(\vec{r})\vec{\nabla}\psi_{\vec{k}}^{(+)}(\vec{r}) - \left(\vec{\nabla}\psi_{\vec{k}}^{(+)*}(\vec{r})\right)\psi_{\vec{k}}^{(+)}(\vec{r})\right]$$

we have

$$\vec{J}\cdot\hat{r} = \frac{\hbar}{2im}\left[\psi_{\vec{k}}^{(+)*}\frac{\partial\psi_{\vec{k}}^{(+)}}{\partial r} - \frac{\partial\psi_{\vec{k}}^{(+)*}}{\partial r}\psi_{\vec{k}}^{(+)}\right].$$

The probability conservation implies

$$0 = \frac{\hbar}{2im}\int_{4\pi} d\Omega\, R^2\left[\psi_{\vec{k}}^{(+)*}\frac{\partial\psi_{\vec{k}}^{(+)}}{\partial r} - \frac{\partial\psi_{\vec{k}}^{(+)*}}{\partial r}\psi_{\vec{k}}^{(+)}\right]\Bigg|_{r=R}.$$

For large values of $R\to\infty$, we can use the asymptotic form of $\psi_{\vec{k}}^{(+)}$ above,

$$\psi_{\vec{k}}^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} \sum_{l=0}^{\infty}(2l+1)i^l P_l(\hat{k}\cdot\hat{r}) \times \frac{1}{2kr}\left[S_l(k)e^{i[kr-(l+1)\frac{\pi}{2}]} + e^{-i[kr-(l+1)\frac{\pi}{2}]}\right]$$

and

$$\frac{\partial \psi^{(+)}_{\vec{k}}(\vec{r})}{\partial r} \underset{r\to\infty}{\sim} \sum_{l=0}^{\infty} (2l+1)\, i^{l} P_l(\hat{k}\cdot\hat{r}) \frac{i}{2r} \times$$

$$\times \Big\{ \Big[S_l(k)\, e^{i[kr-(l+1)\frac{\pi}{2}]} - e^{-i[kr-(l+1)\frac{\pi}{2}]} \Big]$$

$$+ \underbrace{\frac{i}{kr}\Big(S_l(k)\, e^{i[kr-(l+1)\frac{\pi}{2}]} + e^{-i[kr-(l+1)\frac{\pi}{2}]} \Big)}_{\text{for } r\to\infty \text{ this is negligible compared to the first term}} \Big\}$$

Thus we find, using $P_l^{*}(\hat{k}\cdot\hat{r}) = P_l(\hat{k}\cdot\hat{r})$,

$$0 = \int_{4\pi} d\Omega\, R^2 \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)(-i)^{l} (2l'+1)\, i^{l'} P_l(\hat{k}\cdot\hat{r}) P_{l'}(\hat{k}\cdot\hat{r})$$

$$\Big\{ \frac{i}{4kR^2} \Big[S_l^{*}(k)\, e^{-i[kR-(l+1)\frac{\pi}{2}]} + e^{+i[kR-(l+1)\frac{\pi}{2}]} \Big] \times$$

$$\times \Big[S_{l'}(k)\, e^{+i[kR-(l'+1)\frac{\pi}{2}]} - e^{-i[kR-(l'+1)\frac{\pi}{2}]} \Big]$$

$$+ \frac{i}{4kR^2} \Big[S_l^{*}(k)\, e^{-i[kR-(l+1)\frac{\pi}{2}]} - e^{+i[kR-(l+1)\frac{\pi}{2}]} \Big] \times$$

$$\times \Big[S_{l'}(k)\, e^{+i[kR-(l'+1)\frac{\pi}{2}]} + e^{-i[kR-(l'+1)\frac{\pi}{2}]} \Big] \Big\}$$

Now
$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}\cdot\hat{r})\, P_l(\hat{k}\cdot\hat{r}) = \frac{4\pi}{2l+1}\,\delta_{ll'},$$

hence

$$0 = \frac{i}{4k}\sum_{l=0}^{\infty}(2l+1)\,4\pi\Big\{\Big[S_l^*(k)\,e^{-i[kR-(l+1)\frac{\pi}{2}]} + e^{+i[kR-(l+1)\frac{\pi}{2}]}\Big]\times$$
$$\times\Big[S_l(k)\,e^{+i[kR-(l+1)\frac{\pi}{2}]} - e^{-i[kR-(l+1)\frac{\pi}{2}]}\Big]$$
$$+\Big[S_l^*(k)\,e^{-i[kR-(l+1)\frac{\pi}{2}]} - e^{+i[kR-(l+1)\frac{\pi}{2}]}\Big]\times$$
$$\times\Big[S_l(k)\,e^{+i[kR-(l+1)\frac{\pi}{2}]} + e^{-i[kR-(l+1)\frac{\pi}{2}]}\Big]\Big\}$$

$$= \frac{i\pi}{k}\sum_{l=0}^{\infty}(2l+1)\Big\{\big(|S_l(k)|^2-1\big)2$$
$$\cancel{-S_l^*(k)\,e^{-2i[kR-(l+1)\frac{\pi}{2}]}} + \cancel{S_l(k)\,e^{+2i[kR-(l+1)\frac{\pi}{2}]}}$$
$$\cancel{+S_l^*(k)\,e^{-2i[kR-(l+1)\frac{\pi}{2}]}} - \cancel{S_l(k)\,e^{+2i[kR-(l+1)\frac{\pi}{2}]}}\Big\}$$

The cross-terms cancel, and we finally obtain the conservation of probability

$$\boxed{0 = \sum_{l=0}^{\infty} (2l+1)\left(|S_l(k)|^2 - 1\right)}$$

$|S_l(k)| = 1$ is sufficient for this equation to be satisfied but not necessary, there can be cancellations between terms. However, since the Schrödinger equation is linear, the principle of superposition is valid.

Given two solutions $\psi^{(+)}_{\vec{k}_1}$, $\psi^{(+)}_{\vec{k}_2}$ with $|\vec{k}_1| = |\vec{k}_2| = k$, then $\psi^{(+)}(\vec{r}) = \alpha\psi^{(+)}_{\vec{k}_1}(\vec{r}) + \beta\psi^{(+)}_{\vec{k}_2}(\vec{r})$ with $\alpha, \beta \in \mathbb{C}$, is a stationary state with the same energy. It represents two waves moving in different directions. Since $\psi^{(+)}(\vec{r})$ is time independent, the probability density is independent of time also, and we can repeat all of the above analysis using $\psi^{(+)}(\vec{r})$ instead of $\psi^{(+)}_{\vec{k}}(\vec{r})$.

The asymptotic form of $\psi^{(+)}(\vec{r})$ is

$$\psi^{(+)}(\vec{r}) \underset{r\to\infty}{\sim} \sum_{l=0}^{\infty}(2l+1)i^l\frac{1}{2kr}\left[S_l(k)e^{i[kr-(l+1)\frac{\pi}{2}]} + e^{-i[kr-(l+1)\frac{\pi}{2}]}\right]\times$$

$$\times\left(\alpha P_l(\hat{k}_1\cdot\hat{r}) + \beta P_l(\hat{k}_2\cdot\hat{r})\right)$$

and so

$$\frac{\partial\psi^{(+)}(\vec{r})}{\partial r} \underset{r\to\infty}{\sim} \sum_{l=0}^{\infty}(2l+1)i^l\frac{i}{2r}\left[S_l(k)e^{i[kr-(l+1)\frac{\pi}{2}]} - e^{-i[kr-(l+1)\frac{\pi}{2}]}\right]\times$$

$$\times\left(\alpha P_l(\hat{k}_1\cdot\hat{r}) + \beta P_l(\hat{k}_2\cdot\hat{r})\right).$$

Substituting into the probability conservation equation,

$$0 = \oint_S d\vec{S}\cdot\vec{J}$$

we have 4 different angular integrals to perform due to the $(\alpha P_l(\hat{k}_1\cdot\hat{r}) + \beta P_l(\hat{k}_2\cdot\hat{r}))$ products

That is we must evaluate

$$\int_{4\pi} d\Omega \left[\alpha^* P_{l'}(\hat{k}_1\cdot\hat{r}) + \beta^* P_{l'}(\hat{k}_2\cdot\hat{r})\right]\left[\alpha P_l(\hat{k}_1\cdot\hat{r}) + \beta P_l(\hat{k}_2\cdot\hat{r})\right]$$

$$= |\alpha|^2 \int_{4\pi} d\Omega\, P_{l'}(\hat{k}_1\cdot\hat{r}) P_l(\hat{k}_1\cdot\hat{r})$$

$$+ |\beta|^2 \int_{4\pi} d\Omega\, P_{l'}(\hat{k}_2\cdot\hat{r}) P_l(\hat{k}_2\cdot\hat{r})$$

$$+ \alpha^*\beta \int_{4\pi} d\Omega\, P_{l'}(\hat{k}_1\cdot\hat{r}) P_l(\hat{k}_2\cdot\hat{r})$$

$$+ \alpha\beta^* \int_{4\pi} d\Omega\, P_{l'}(\hat{k}_2\cdot\hat{r}) P_l(\hat{k}_1\cdot\hat{r}) .$$

The first 2-integrals are straightforward

$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}_1\cdot\hat{r}) P_l(\hat{k}_1\cdot\hat{r}) = \int_{4\pi} d\Omega\, P_{l'}(\hat{k}_2\cdot\hat{r}) P_l(\hat{k}_2\cdot\hat{r}) = \frac{4\pi\,\delta_{ll'}}{2l+1}$$

The 2-cross term integrals require the use of the addition theorem for spherical harmonics

$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}_1\cdot\hat{r})\, P_l(\hat{k}_2\cdot\hat{r})$$

$$= \frac{(4\pi)^2}{(2l+1)(2l'+1)} \sum_{m=-l}^{+l} \sum_{m'=-l'}^{+l'} \int_{4\pi} d\Omega \,\times$$

$$\times\, Y_l^m(\theta_{\vec{k}_1}, \varphi_{\vec{k}_1})\, Y_l^{m*}(\theta,\varphi)\, Y_{l'}^{m'}(\theta,\varphi)\, Y_{l'}^{m'*}(\theta_{\vec{k}_2}, \varphi_{\vec{k}_2})$$

But $\int_{4\pi} d\Omega\, Y_l^{m*}(\theta,\varphi)\, Y_{l'}^{m'}(\theta,\varphi) = \delta_{ll'}\,\delta_{mm'}$

Thus we find

$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}_1\cdot\hat{r})\, P_l(\hat{k}_2\cdot\hat{r}) = \delta_{ll'} \frac{(4\pi)^2}{(2l+1)^2} \,\times$$

$$\times \sum_{m=-l}^{+l} Y_l^m(\theta_{\vec{k}_1}, \varphi_{\vec{k}_1})\, Y_l^{m*}(\theta_{\vec{k}_2}, \varphi_{\vec{k}_2})$$

Using the addition theorem inreverse now

$$= \frac{4\pi}{(2l+1)} \delta_{ll'}\, P_l(\hat{k}_1\cdot\hat{k}_2).$$

Similarly for the other crossterm

$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}_2\cdot\hat{r})P_l(\hat{k}_1\cdot\hat{r}) = \frac{4\pi}{(2l+1)}\delta_{ll'}P_l(\hat{k}_1\cdot\hat{k}_2)$$

Putting this altogether we find for the angular integrals

$$\int_{4\pi} d\Omega\left[\alpha^* P_{l'}(\hat{k}_1\cdot\hat{r}) + \beta^* P_{l'}(\hat{k}_2\cdot\hat{r})\right]\left[\alpha P_l(\hat{k}_1\cdot\hat{r}) + \beta P_l(\hat{k}_2\cdot\hat{r})\right]$$

$$= \frac{4\pi}{(2l+1)}\delta_{ll'}\left[|\alpha|^2 + |\beta|^2 + (\alpha^*\beta + \alpha\beta^*)P_l(\hat{k}_1\cdot\hat{k}_2)\right]$$

Hence in the continuity equation this factor replaces the previous integral of

$$\int_{4\pi} d\Omega\, P_{l'}(\hat{k}\cdot\hat{r})P_l(\hat{k}\cdot\hat{r}) = \frac{4\pi}{(2l+1)}\delta_{ll'}.$$

Thus we find

$$\boxed{0 = \sum_{l=0}^{\infty}(2l+1)\left(|S_l(k)|^2 - 1\right)\times \left[|\alpha|^2 + |\beta|^2 + (\alpha^*\beta + \alpha\beta^*)P_l(\hat{k}_1\cdot\hat{k}_2)\right]}$$

Since the $P_\ell(\hat{k}_1 \cdot \hat{k}_2)$ are linearly independent and α and β are arbitrary (except for the overall normalization $|\alpha|^2+|\beta|^2=1$) the coefficient of $P_\ell(\hat{k}_1 \cdot \hat{k}_2)$ must vanish for each ℓ if the sum is to vanish. Thus we obtain

$$|S_\ell(k)|^2 = 1 \qquad \text{for each } \ell$$

and so

$$S_\ell(k) = e^{2i\delta_\ell(k)} \qquad \text{with } \delta_\ell(k) \in \mathbb{R}.$$

Thus we find that (page -1065-) the scattering amplitude for real potential scattering is

$$f^{(+)}(\vec{k},\vec{k}') = \sum_{l=0}^{\infty} (2\ell+1)\left[\frac{S_\ell(k)-1}{2ik}\right] P_\ell(\hat{k}\cdot\hat{k}')$$

$$= \sum_{l=0}^{\infty} (2\ell+1)\left[\frac{e^{2i\delta_\ell}-1}{2ik}\right] P_\ell(\hat{k}\cdot\hat{k}')$$

$$= \sum_{l=0}^{\infty} (2\ell+1)\frac{e^{i\delta_\ell}\sin\delta_\ell}{k} P_\ell(\hat{k}\cdot\hat{k}') .$$

The differential cross-section is given by

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

$$= \left| \sum_{l=0}^{\infty}{}' (2l+1) \frac{e^{i\delta_l}\sin\delta_l}{k} P_l(\hat{k}\cdot\hat{k}') \right|^2$$

and the total cross-section is the integral of this over all solid angles

$$\sigma_{elastic} = \int_{4\pi} d\Omega\, \sigma(\theta,\varphi)$$

$$= \int_{4\pi} d\Omega \sum_{l=0}^{\infty}{}' \sum_{l'=0}^{\infty}{}' (2l+1)(2l'+1) \frac{e^{-i\delta_l} e^{+i\delta_{l'}}}{k^2} \times$$

$$\times \sin\delta_{l'} \sin\delta_l\, P_l(\hat{k}\cdot\hat{k}') P_{l'}(\hat{k}\cdot\hat{k}')$$

as usual

$$\int_{4\pi} d\Omega\, P_l(\hat{k}\cdot\hat{k}') P_{l'}(\hat{k}\cdot\hat{k}')$$

$$= \int_{4\pi} d\Omega\, P_l(\hat{k}\cdot\hat{r}) P_{l'}(\hat{k}\cdot\hat{r})$$

$$= \frac{4\pi}{(2l+1)} \delta_{ll'}$$

Thus the total elastic scattering cross section becomes

$$\sigma_{elastic} = 4\pi \sum_{l=0}^{\infty} (2l+1) \frac{\sin^2\delta_l}{k^2} \quad .$$

Defining the contribution to $\sigma_{elastic}$ from the l^{th} partial wave as

$$\sigma_{elastic}^{(l)}(k) \equiv 4\pi (2l+1) \frac{\sin^2\delta_l(k)}{k^2}$$

so that

$$\sigma_{elastic} = \sum_{l=0}^{\infty} \sigma_{elastic}^{(l)}(k) \quad ,$$

we see that for each l (and k), there is a maximum value for $\sigma_{elastic}^{(l)}(k)$

$$\sigma_{\substack{elastic\\max}}^{(l)}(k) = \frac{4\pi(2l+1)}{k^2} \quad .$$

This is the maximum contribution from the l^{th} partial wave to the total elastic cross-section.

Finally, in the special case where $\vec{k}' = \vec{k}$, the forward elastic scattering case, the scattering amplitude becomes

$$f^{(+)}(\vec{k},\vec{k}) = \sum_{l=0}^{\infty}{}' (2l+1) \frac{e^{i\delta_l}\sin\delta_l}{k} \underbrace{P_l(\hat{k}\cdot\hat{k})}_{=P_l(1)=1}$$

$$= \sum_{l=0}^{\infty}{}' (2l+1) \frac{e^{i\delta_l}\sin\delta_l}{k} .$$

Thus

$$\operatorname{Im} f^{(+)}(\vec{k},\vec{k}) = \sum_{l=0}^{\infty}{}' (2l+1) \frac{\sin^2\delta_l}{k}$$

$$= \frac{k}{4\pi}\sigma_{\text{elastic}} ,$$

that is

$$\boxed{\sigma_{\text{elastic}} = \frac{4\pi}{k} \operatorname{Im} f^{(+)}(\vec{k},\vec{k}) .}$$

The total cross-section is $\frac{4\pi}{k}$ times the imaginary part of the forward elastic scattering amplitude. This result is known as the Optical Theorem.