Partial wave expansion and Geen's function

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To speak roughly, the Born approximation may be useful when the energy of the incident particle is high. There is another approach, known as the partial wave expansion (or partial phase shift), that is most useful at low energies and is somewhat complementary to the Born approximation.

Rayleigh's expansion
Optical theorem
Phase shift

1 Introduction

We now look for the solution of the Schrödinger equation for a particle in the presence of potential energy $V(r)$ (with spherical symmetry)

$$\psi_{klm} = R_{kl}(r) Y_l^m(\theta,\phi),$$

and

$$R_{kl}(r) = \frac{u_{kl}(r)}{r}$$

with

$$[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)]R_{kl}(r) = ER_{kl}(r)$$

or

$$[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)]R_{kl}(r) = ER_{kl}(r) = \frac{\hbar^2}{2\mu}k^2 R_{kl}(r)$$

or

$$\frac{d^2}{dr^2}[rR_{kl}(r)] + [k^2 - \frac{l(l+1)}{r^2} - U(r)]rR_{kl}(r) = 0$$

where

$$U(r) = \frac{2\mu}{\hbar^2}V(r), \qquad E = \frac{\hbar^2}{2\mu}k^2$$

Fig.

$$p_r{}^2 R_{kl}(r) = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}(rR_{kl}(r)) = -\hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2}(rR_{kl}(r))$$

and μ is a reduced mass. Then $u_{kl}(r) = rR_{kl}(r)$ satisfies the differential equation

$$\frac{d^2}{dr^2}u_{kl}(r) + [k^2 - \frac{l(l+1)}{r^2} - U(r)]u_{kl}(r) = 0.$$

(i) Case-1

The radial equation for the external region $r>a$, where the scattering potential vanishes, is equal to

$$\frac{d^2}{dr^2}u_{kl}(r) + [k^2 - \frac{l(l+1)}{r^2}]u_{kl}(r) = 0.$$

where

$$U(r) = 0.$$

The solution of $R_{kl}(r)$ is

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \alpha_l j_l(kr) + \beta_l n_l(kr) \qquad \text{for } r>a \text{ (radiation zone)}$$

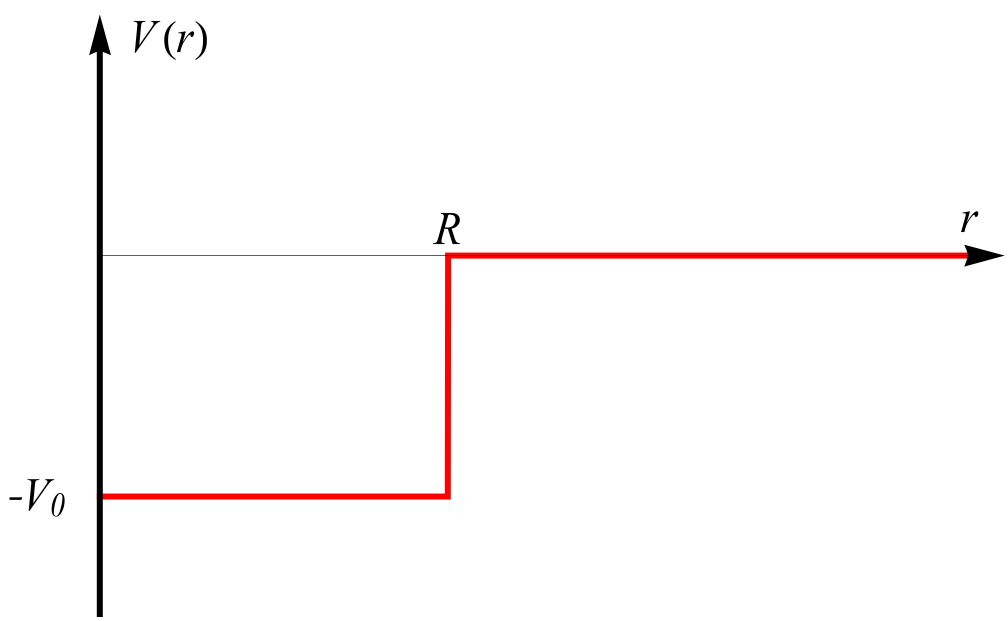


Fig. Attractive potential, which becomes zero for $r \to \infty$.

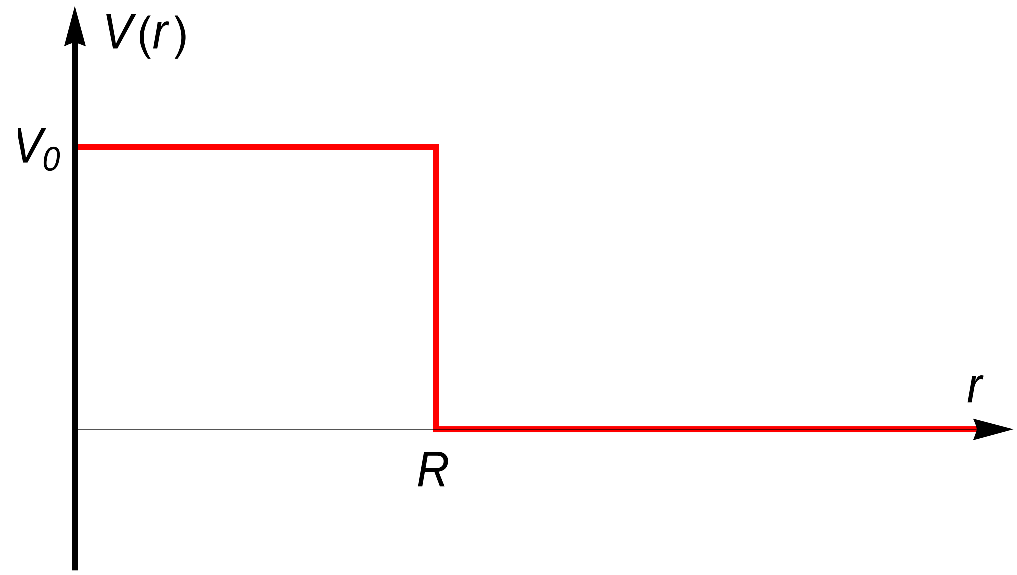


Fig. Repulsive potential which becomes zero for $r \to \infty$.

(ii) Case-2 (free particle)

In the complete absence of a scattering potential ($V = 0$ everywhere),

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \gamma_l j_l(kr)$$

The condition of the normalization:

$$4\pi\gamma_l^2 \int_0^\infty dr r^2 [j_l(kr)]^2 = 1$$

2. Semi-classical argument for the angular momentum,

((Classical mechanics))

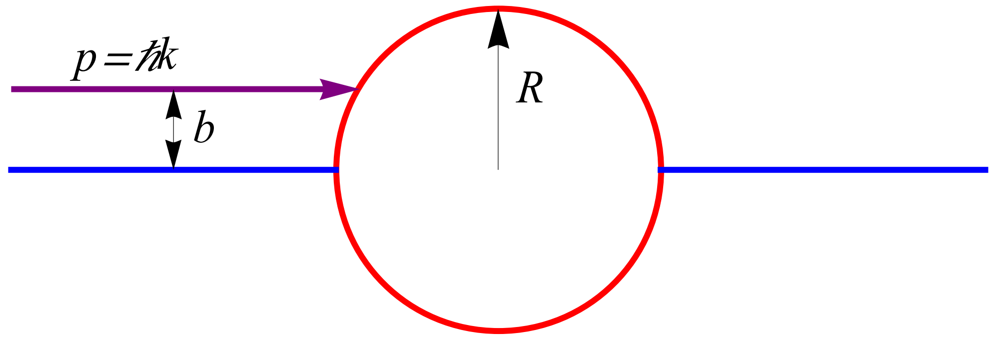
The particles with the impact parameter b possesses the angular momentum L given by

$$L = pb\,,$$

where p $(=\hbar k)$ is the linear momentum of the particles. Only particles with impact parameter b less than or equal to the range R of the potential energy would interact with the target;

$$L \leq L_{\max} = \hbar kR$$

since b<R.



When energy is low, L_{max} is small. Partial waves for higher l are, in general, unimportant. That is why the partial wave expansion is useful in the case of low energy incident particle. The main contribution to the scattering is the S-wave (l = 0). The P-wave (l = 1) does not contribute in typical cases.

((**Quantum mechanics**))

In quantum mechanics, we have

$$L = \hbar\sqrt{l(l+1)} \approx \hbar l\,, \qquad\qquad p = \hbar k$$

The potential of interaction is appreciable only over the range r_0. If $s > r_0$, the interaction is negligible,

$$\frac{l}{p} = s > r_0$$

or

$$\frac{\hbar l}{\hbar k} > r_0 \qquad \text{or} \qquad l > r_0 k$$

where s is comparable to the impact parameter b in the classical mechanics. The partial waves with ***l*** values in excess of $r_0 k$ will suffer little or no shift in phase.

3. Asymptotic form

Far from the interaction point, where the potential is negligible, the scattered wave function has the general form

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = \alpha_l j_l(kr) + \beta_l n_l(kr)$$

since the position of the particle is far from the origin, where the function $n_l(kr)$ is poorly behaved. We use

$$\alpha_l = a_l \cos\delta_l, \qquad \beta_l = -a_l \sin\delta_l .$$

Then we have

$$\begin{aligned} R_{kl}(r) &= a_l[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)] \\ &= a_l \cos\delta_l [j_l(kr) - \tan\delta_l n_l(kr)] \end{aligned}$$

Note that $\delta_l = 0$ for free particle (the case-2). Since

$$j_l(kr) \to \frac{\sin(kr - \frac{l\pi}{2})}{kr}, \qquad n_l(kr) \to -\frac{\cos(kr - \frac{l\pi}{2})}{kr}$$

as $r \to \infty$, then we have

$$\begin{aligned} R_{kl}(r) &= \frac{a_l \cos\delta_l \sin(kr - \frac{l\pi}{2})}{kr} + \frac{a_l \cos\delta_l \cos(kr - \frac{l\pi}{2})}{kr} \\ &= a_l \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \end{aligned}$$

or

$$R_{kl}(r) = a_l \frac{e^{-i\delta_l}[e^{i(kr - \frac{l\pi}{2} + 2\delta_l)} - e^{-i(kr - \frac{l\pi}{2})}]}{2ikr}$$

Suppose that the scattering amplitude $\psi^{(+)}(r,\theta)$ is independent of ϕ. Since

$$L_z\psi^{(+)} = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\psi^{(+)} = m\hbar\psi^{(+)} = 0,$$

the magnetic quantum number m should be equal to zero. Thus we have

$$\psi^{(+)}(r,\theta) = \sum_l c_l R_{kl}(r) Y_l^{m=0}(\theta,\phi)$$

$$= \sum_l c_l \sqrt{\frac{2l+1}{4\pi}} R_{kl}(r) P_l(\cos\theta)$$

$$= \sum_l \frac{c_l a_l i^{-l}}{\sqrt{4\pi(2l+1)}} e^{-i\delta_l} i^l \frac{2l+1}{2i} \frac{[e^{i(kr-\frac{l\pi}{2}+2\delta_l)} - e^{-i(kr-\frac{l\pi}{2})}]}{kr} P_l(\cos\theta)$$

where c_l is constant. Note that

$$Y_l^{m=0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) .$$

The complete solution of the scattering wave function is

$$\psi^{(+)}(r,\theta) = \sum_{l=0}^{\infty} a_l \frac{i^l (2l+1)\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} P_l(\cos\theta)$$
$$= \sum_{l=0}^{\infty} a_l e^{-i\delta_l} i^l \left(\frac{2l+1}{2i}\right) \frac{1}{kr} [e^{i(kr-\frac{l\pi}{2}+2\delta_l)} - e^{-i(kr-\frac{l\pi}{2})}] P_l(\cos\theta) \qquad (1)$$

where the replacement of the coefficient is made as

$$\frac{c_l a_l i^{-l}}{\sqrt{4\pi(2l+1)}} \rightarrow a_l .$$

((**Note**)) Spherical Hankel functions, $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$

$$h_l^{(1)}(x) = j_l(x) + i n_l(x) , \qquad h_l^{(2)}(x) = j_l(x) - i n_l(x) .$$

4. Partial wave expansion of the scattering amplitude

On the other hand, $\psi^{(+)}(r,\theta)$ has the form

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}} [e^{ikz} + \frac{1}{r} e^{ikr} f(\theta)]$$

Note that

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) , \qquad (2)$$

(Rayleigh's expansion)

where we take ***k*** in the *z* axis. Since

$$j_l(kr) \to \frac{\sin(kr - \frac{l\pi}{2})}{kr} \qquad \text{in the limit of } r \to \infty$$

we get

$$e^{ikz} \to \sum_{l=0}^{\infty} \frac{i^l (2l+1)\sin(kr - \frac{l\pi}{2})}{kr} P_l(\cos\theta)$$
$$= \sum_{l=0}^{\infty} i^l \left(\frac{2l+1}{2i}\right) \frac{1}{kr} [e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}] P_l(\cos\theta) .$$

From Eq.(1),

$$\psi^{(+)}(r,\theta) \to \sum_l a_l e^{-i\delta_l} i^l \left(\frac{2l+1}{2i}\right) \frac{1}{kr} [e^{i(kr - \frac{l\pi}{2} + 2\delta_l)} - e^{-i(kr - \frac{l\pi}{2})}] P_l(\cos\theta) .$$

From Eq.(2),

$$\psi^{(+)}(r,\theta) \approx e^{ikz} + \frac{1}{r} e^{ikr} f(\theta)$$
$$= \sum_{l=0}^{\infty} \left(\frac{2l+1}{2i}\right) i^l \frac{1}{kr} [e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}] P_l(\cos\theta) + \frac{1}{r} e^{ikr} f(\theta)$$

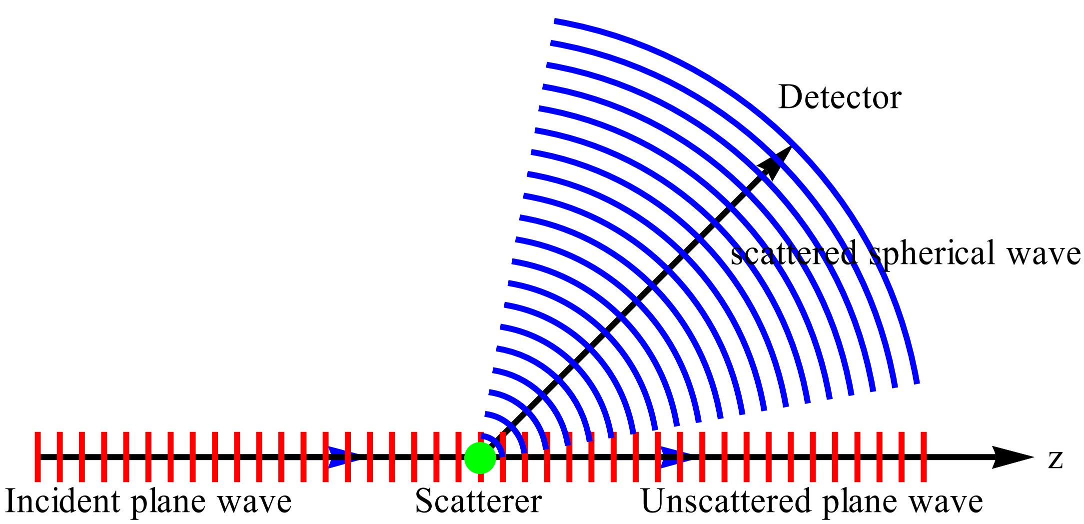


Fig. Schematic layout for scattering experiment. The scattering angle is the laboratory angle.

Therefore we have

$$\frac{1}{r}e^{ikr}f(\theta)=\sum_{l=0}^{\infty}a_l e^{-i\delta_l}i^l\left(\frac{2l+1}{2i}\right)\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2}+2\delta_l)}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$
$$-\sum_{l=0}^{\infty}\left(\frac{2l+1}{2i}\right)i^l\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

The coefficient of the term $e^{-i(kr-\frac{l\pi}{2})}$ is assumed to be equal to zero for the incoming spherical wave. Then we have

$$-a_l e^{-i\delta_l}+1=0$$

or

$$a_l=e^{i\delta_l}\ .$$

Then we get

$$\frac{1}{r}e^{ikr}f(\theta)=\sum_l i^l\left(\frac{2l+1}{2i}\right)\frac{e^{ikr}}{kr}e^{i\delta_l}[e^{i(-\frac{l\pi}{2}+\delta_l)}-e^{i(-\frac{l\pi}{2}-\delta_l)}]P_l(\cos\theta)$$

Noting that

$$i^l=e^{i\frac{\pi l}{2}}$$

we have

$$\frac{1}{r}e^{ikr}f(\theta)=\sum_l e^{i\frac{\pi l}{2}}\left(\frac{2l+1}{2i}\right)\frac{e^{ikr}}{kr}e^{i\delta_l}[e^{i(-\frac{l\pi}{2}+\delta_l)}-e^{i(-\frac{l\pi}{2}-\delta_l)}]P_l(\cos\theta)$$
$$=\sum_l\left(\frac{2l+1}{2i}\right)\frac{e^{ikr}}{kr}e^{i\delta_l}(e^{i\delta_l}-e^{-i\delta_l})P_l(\cos\theta)$$
$$=\frac{e^{ikr}}{r}\sum_l(2l+1)\frac{1}{k}e^{i\delta_l}\sin(\delta_l)P_l(\cos\theta)$$

or

$$f(\theta)=\sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta),$$

with

$$f_l(k)=\frac{1}{k}e^{i\delta_l}\sin(\delta_l), \qquad \mathrm{Im}\, f_l(k)=\frac{1}{k}\sin^2(\delta_l)$$

or

$$kf_l(k)=e^{i\delta_l}\frac{1}{2i}(e^{i\delta_l}-e^{-i\delta_l})=\frac{1}{2i}(e^{2i\delta_l}-1)=\frac{i}{2}(1-e^{2i\delta_l}).$$

$f_l(k)$ is defined by

$$f_l(k)=\frac{1}{2ik}(e^{2i\delta_l}-1)=\frac{1}{2ik}[S_l(k)-1],$$

where $S_l(k)$ is the phase shift given by

$$S_l(k)=e^{2i\delta_l}$$

The total cross section is given by

$$\sigma_{tot}=\int |f(\theta)|^2 d\Omega$$

where $d\Omega=2\pi\sin\theta d\theta$

$$|f(\theta)|^2=\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)f_l^*(k)f_{l'}(k)P_l(\cos\theta)P_{l'}(\cos\theta)$$

Noting that

$$\int d\Omega P_l(\cos\theta)P_{l'}(\cos\theta)=\frac{4\pi}{2l+1}\delta_{l,l'},$$

we have

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

where

$$|f_l(k)|^2 = \frac{1}{k^2}\sin^2\delta_l$$

((**D. Bohm, Quantum Theory p.564**))

This formula yields the angular-dependent cross section, once we know δ_l. The value of δ_l must be obtained by solving the Schrödinger's equation. The angular dependence arises, in part, from the interference of waves of different *l*.

5. Optical theorem

We can check the optical theorem. We start with the expression of $f(\theta)$,

$$\begin{aligned} f(\theta) &= \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta) \\ &= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin(\delta_l)P_l(\cos\theta) \\ &= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\cos(\delta_l)\sin(\delta_l)P_l(\cos\theta) + \frac{i}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)P_l(\cos\theta) \end{aligned}$$

Then we have

$$\begin{aligned} \mathrm{Im}[f(\theta=0)] &= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)P_l(\cos\theta)\,|_{\theta=0} \\ &= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l) \end{aligned}$$

where

$$P_l(\cos\theta)\,|_{\theta=0} = 1.$$

This means that

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

What this theorem means? The probability conservation requirement indicates that the amplitude of the incident wave ($\frac{\hbar k}{m}$) must ultimately be reduced in proportion to the total probability that the particle is scattered in any way [$(\hbar k/m)\sigma_{tot}$].

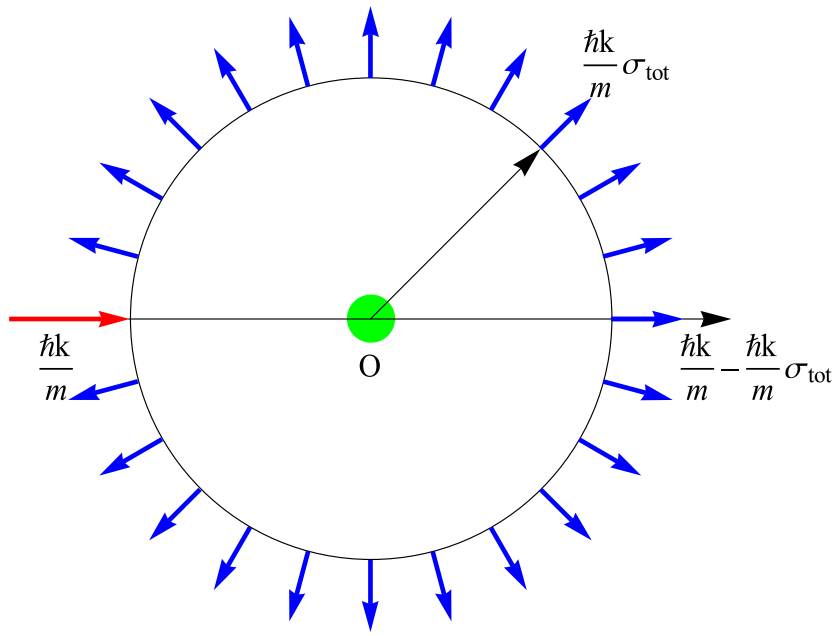


Fig. **Optical theorem**. The intensity of the incident wave is $\hbar k/m$. The intensity of the forward wave is $(\hbar k/m)-(4\pi\hbar/m)\mathrm{Im}[f(0)]$. The waves with the total intensity $(4\pi\hbar/m)\mathrm{Im}[f(0)]=(\hbar k/m)\sigma_{tot}$ is scattered for all the directions, as the scattering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

When scattering occurs, part of the energy carried by the incident wave is radiated into all angles. This energy must be removed from the incident wave. Consequently the energy flowing in the forward direction is reduced and this modifies the scattering amplitude in the forward direction ($\theta = 0$).

We now consider the complex plane

$$z \equiv kf_l(k) = e^{i\delta_l}\sin(\delta_l) = \frac{1}{2i}(e^{2i\delta_l}-1) = \frac{i}{2}+\frac{1}{2}e^{i(2\delta_l-\frac{\pi}{2})}$$

or

$$z-\frac{i}{2}=\frac{1}{2}e^{i(2\delta_l-\frac{\pi}{2})}$$

This is a circle of radius 1/2 centered at (i/2) in the complex plane.

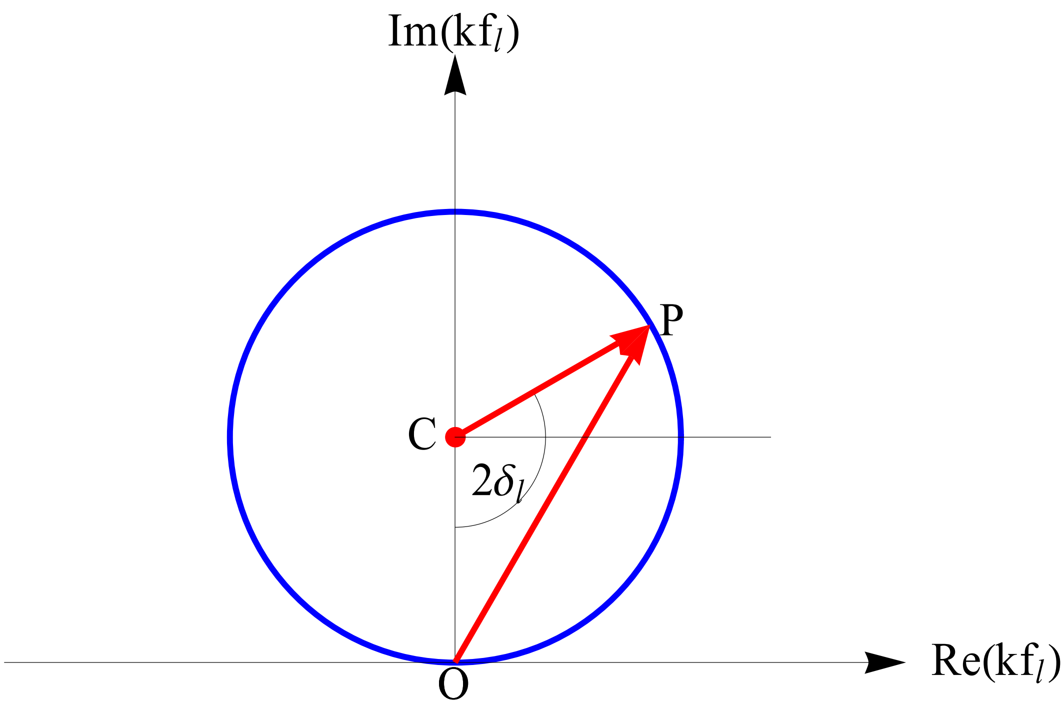


Fig. Argand diagram of $z = kf_l(k)$; The circle is called the *unitary circle*.

$$OP = k\left|f_l(k)\right|, \qquad \overline{OC} = 1/2, \qquad \overline{CP} = 1/2$$
$$\angle OCP = 2\delta_l$$

(i) $\delta_l \approx 0$

kf_l must stay near the bottom of the circle. kf_l may be positive or negative, but kf_l is almost purely real.

$$kf_l(k) = e^{i\delta_l}\sin(\delta_l) \approx \delta_l .$$

(ii) $\delta_l \approx \pi/2$

kf_l is almost purely imaginary and kf_l is maximal. Under such a condition the *l*-th partial wave may be in resonance.

$$kf_l(k) = e^{i\frac{\pi}{2}} = i .$$

$$\sigma_{tot}^{(l)} = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}(2l+1).$$

6. Expression of the Forward scattering (based on the book of Gasiorowicz)

We show that the forward scattering is expressed by

$$\frac{\hbar k}{m} - \frac{4\pi\hbar}{m}\mathrm{Im}[f(0)]$$

((**Proof**))
We start with the wave function

$$\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\theta)$$

Probability current density is given by

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{\hbar}{2im}[\psi^*(\boldsymbol{r})\nabla\psi(\boldsymbol{r}) - \psi(\boldsymbol{r})\nabla\psi^*(\boldsymbol{r})]$$

with

$$\nabla = \boldsymbol{e}_r\frac{\partial}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \boldsymbol{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

Thus we have

$$\begin{aligned}
\boldsymbol{j}(\boldsymbol{r}) &= \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r}f^*(\theta)]\nabla[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\theta)] + c.c. \\
&= \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r}f^*(\theta)][\boldsymbol{e}_r\frac{\partial}{\partial r}(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\theta)) + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r}f(\theta))] + c.c \\
&= \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r}f^*(\theta)][i\boldsymbol{e}_r(k\cos\theta)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_r f(\theta)\frac{\partial}{\partial r}\frac{e^{ikr}}{r} + \boldsymbol{e}_\theta(-ik\sin\theta)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_\theta\frac{e^{ikr}}{r^2}\frac{\partial}{\partial\theta}f(\theta)]] + c.c.
\end{aligned}$$

where $\boldsymbol{k}\cdot\boldsymbol{r} = kr\cos\theta$

$$\frac{\partial}{\partial r}\frac{e^{ikr}}{r} = \frac{ikre^{ikr} - e^{ikr}}{r^2} = (\frac{ikr-1}{r^2})e^{ikr},$$

This can be rewritten as

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r} f^*(\theta)]\nabla[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r} f(\theta)] + c.c.$$
$$= \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r} f^*(\theta)][\boldsymbol{e}_r \frac{\partial}{\partial r}(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r} f(\theta)) + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{ikr}}{r} f(\theta))] + c.c$$
$$= \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r} f^*(\theta)][i\boldsymbol{e}_r(k\cos\theta)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_r f(\theta)\frac{\partial}{\partial r}\frac{e^{ikr}}{r} + \boldsymbol{e}_\theta(-ik\sin\theta)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_\theta \frac{e^{ikr}}{r^2}\frac{\partial}{\partial\theta} f(\theta)]] + c.c$$

or

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{\hbar}{2im}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{e^{-ikr}}{r} f^*(\theta)][i\boldsymbol{e}_r k\cos\theta e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_r f(\theta)(\frac{ikr-1}{r^2})e^{ikr} + \boldsymbol{e}_\theta(-ik\sin\theta)e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + \boldsymbol{e}_\theta \frac{e^{ikr}}{r^2}\frac{\partial}{\partial\theta} f(\theta)] + c.c$$
$$= \frac{\hbar}{2im}[i\boldsymbol{e}_r(k\cos\theta) + \boldsymbol{e}_r f(\theta)(\frac{ikr-1}{r^2})e^{ikr(1-\cos\theta)} + \boldsymbol{e}_\theta(-ik\sin\theta) + \boldsymbol{e}_\theta \frac{e^{ikr(1-\cos\theta)}}{r^2}\frac{\partial}{\partial\theta} f(\theta)$$
$$+ i\boldsymbol{e}_r k\cos\theta \frac{e^{-ikr(1-\cos\theta)}}{r} f^*(\theta) + \boldsymbol{e}_r(\frac{ikr-1}{r^3}) f(\theta) f^*(\theta) + \boldsymbol{e}_\theta(-ik\sin\theta)\frac{e^{-ikr(1-\cos\theta)}}{r} f^*(\theta) + \boldsymbol{e}_\theta \frac{1}{r^3} f^*(\theta)\frac{\partial}{\partial\theta} f(\theta)]$$
$$+ c.c$$
$$\approx \frac{\hbar}{2im}[ik(\boldsymbol{e}_r\cos\theta - \boldsymbol{e}_\theta\sin\theta) + ik(\boldsymbol{e}_r\cos\theta - \boldsymbol{e}_\theta\sin\theta) f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r} + ik\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r} + ik\boldsymbol{e}_r(\frac{1}{r^2})|f(\theta)|^2$$
$$- \boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r^2} + \boldsymbol{e}_\theta \frac{\partial f(\theta)}{\partial\theta}\frac{e^{ikr(1-\cos\theta)}}{r^2}] + c.c$$
$$= \frac{\hbar}{2im}[i\boldsymbol{k} + i\boldsymbol{k} f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r} + ik\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r} + ik\boldsymbol{e}_r|f(\theta)|^2\frac{1}{r^2}$$
$$- \boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r^2} + \boldsymbol{e}_\theta \frac{\partial f(\theta)}{\partial\theta}\frac{e^{ikr(1-\cos\theta)}}{r^2}] + c.c$$

to the order of $\frac{1}{r^2}$, where

$$k(\boldsymbol{e}_r\cos\theta - \boldsymbol{e}_\theta\sin\theta) = \boldsymbol{k}$$

Thus we have

$$
\begin{aligned}
\boldsymbol{j}(\boldsymbol{r}) &= \frac{\hbar}{2m}[\boldsymbol{k}+\boldsymbol{k}\, f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r}+k\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r}+k\boldsymbol{e}_r\left|f(\theta)\right|^2\frac{1}{r^2} \\
&\quad +i\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r^2}-i\boldsymbol{e}_\theta\frac{\partial f(\theta)}{\partial\theta}\frac{e^{ikr(1-\cos\theta)}}{r^2}] \\
&\quad +\frac{\hbar}{2m}[\boldsymbol{k}+\boldsymbol{k}\, f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r}+k\boldsymbol{e}_r f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r}+k\boldsymbol{e}_r\left|f(\theta)\right|^2\frac{1}{r^2} \\
&\quad -i\boldsymbol{e}_r f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r^2}+i\boldsymbol{e}_\theta\frac{\partial f^*(\theta)}{\partial\theta}\frac{e^{-ikr(1-\cos\theta)}}{r^2}] \\
&= \frac{\hbar}{2m}[2\boldsymbol{k}+\boldsymbol{k}\, f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r}+\boldsymbol{k}\, f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r} \\
&\quad +k\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r}+k\boldsymbol{e}_r f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r} \\
&\quad 2k\boldsymbol{e}_r\left|f(\theta)\right|^2\frac{1}{r^2}+i\boldsymbol{e}_r f(\theta)\frac{e^{ikr(1-\cos\theta)}}{r^2}-i\boldsymbol{e}_r f^*(\theta)\frac{e^{-ikr(1-\cos\theta)}}{r^2} \\
&\quad -i\boldsymbol{e}_\theta\frac{\partial f(\theta)}{\partial\theta}\frac{e^{ikr(1-\cos\theta)}}{r^2}+i\boldsymbol{e}_\theta\frac{\partial f^*(\theta)}{\partial\theta}\frac{e^{-ikr(1-\cos\theta)}}{r^2}]
\end{aligned}
$$

((**Note**)) The above calculations can be calculated using Mathematica (Vector analysis)

$\boldsymbol{e}_r$ -component:

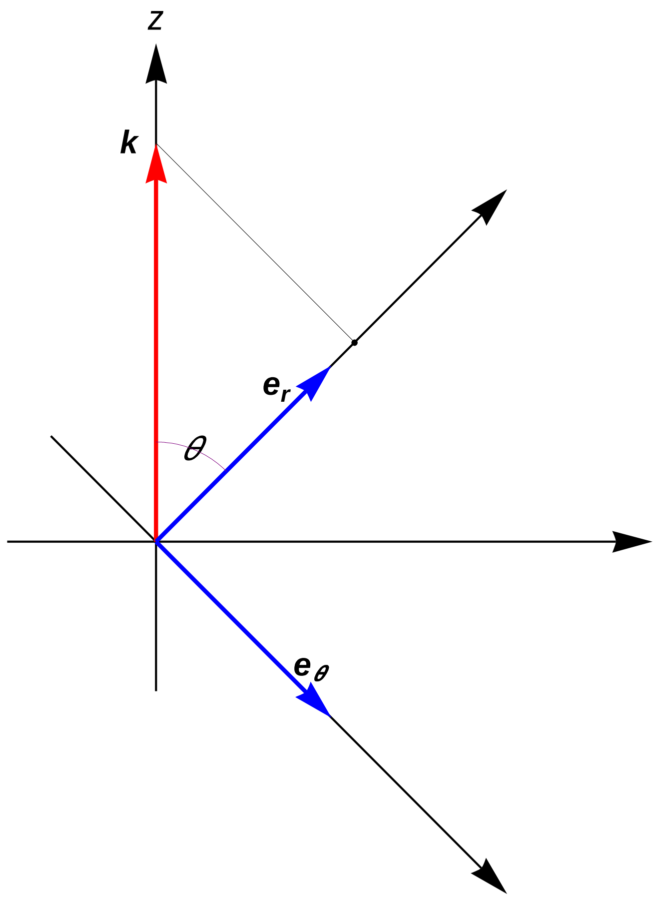
$$
\begin{aligned}
&\boldsymbol{e}_r\frac{\hbar k}{m}\cos\theta+\boldsymbol{e}_r[\frac{i\hbar\, f(\theta)}{2mr^2}e^{ikr(1-\cos\theta)}-\frac{i\hbar\, f^*(\theta)}{2mr^2}e^{-ikr(1-\cos\theta)}] \\
&+\boldsymbol{e}_r[\frac{\hbar k\, f(\theta)}{2mr}e^{ikr(1-\cos\theta)}+\frac{\hbar k\, f^*(\theta)}{2mr}e^{-ikr(1-\cos\theta)}] \\
&+\boldsymbol{e}_r[\frac{\hbar k\cos\theta\, f(\theta)}{2mr}e^{ikr(1-\cos\theta)}+\frac{\hbar k\cos\theta\, f^*(\theta)}{2mr}e^{-ikr(1-\cos\theta)}] \\
&+\boldsymbol{e}_r\frac{\hbar k}{mr^2}f(\theta)f^*(\theta)
\end{aligned}
$$

$\boldsymbol{e}_\theta$ -component:

$$
\begin{aligned}
&-\boldsymbol{e}_\theta\frac{\hbar k}{m}\sin\theta-\boldsymbol{e}_\theta[\frac{i\hbar\, f'(\theta)}{2mr^2}e^{ikr(1-\cos\theta)}-\frac{i\hbar\, f^*{}'(\theta)}{2mr^2}e^{-ikr(1-\cos\theta)}] \\
&-\boldsymbol{e}_\theta[\frac{\hbar k\sin\theta\, f(\theta)}{2mr}e^{ikr(1-\cos\theta)}+\frac{\hbar k\sin\theta\, f^*(\theta)}{2mr}e^{-ikr(1-\cos\theta)}] \\
&+\boldsymbol{e}_\theta[-\frac{i\hbar}{2mr^2}f'(\theta)f^*(\theta)+\frac{i\hbar}{2mr^2}f(\theta)f^*{}'(\theta)]
\end{aligned}
$$

We use

$k(\boldsymbol{e}_r \cos\theta - \boldsymbol{e}_\theta \sin\theta) = \boldsymbol{k}$



$$\boldsymbol{e}_r \frac{\hbar k}{m}\cos\theta + \boldsymbol{e}_r[\frac{i\hbar\, f(\theta)}{2mr^2} e^{ikr(1-\cos\theta)} - \frac{i\hbar\, f^*(\theta)}{2mr^2} e^{-ikr(1-\cos\theta)}]$$
$$+\boldsymbol{e}_r[\frac{\hbar k\, f(\theta)}{2mr} e^{ikr(1-\cos\theta)} + \frac{\hbar k\, f^*(\theta)}{2mr} e^{-ikr(1-\cos\theta)}]$$
$$+\boldsymbol{e}_r[\frac{\hbar k \cos\theta\, f(\theta)}{2mr} e^{ikr(1-\cos\theta)} + \frac{\hbar k \cos\theta\, f^*(\theta)}{2mr} e^{-ikr(1-\cos\theta)}] + \boldsymbol{e}_r \frac{\hbar k}{mr^2} f(\theta) f^*(\theta)$$
$$-\boldsymbol{e}_\theta \frac{\hbar k}{m}\sin\theta - \boldsymbol{e}_\theta[\frac{i\hbar\, f'(\theta)}{2mr^2} e^{ikr(1-\cos\theta)} - \frac{i\hbar\, f^{*}{}'(\theta)}{2mr^2} e^{-ikr(1-\cos\theta)}]$$
$$-\boldsymbol{e}_\theta[\frac{\hbar k \sin\theta\, f(\theta)}{2mr} e^{ikr(1-\cos\theta)} + \frac{\hbar k \sin\theta\, f^*(\theta)}{2mr} e^{-ikr(1-\cos\theta)}]$$
$$+\boldsymbol{e}_\theta[-\frac{i\hbar}{2mr^2} f'(\theta) f^*(\theta) + \frac{i\hbar}{2mr^2} f(\theta) f^{*}{}'(\theta)]$$

So we get the final result as

$$
\begin{aligned}
\boldsymbol{J} &= \frac{\hbar\boldsymbol{k}}{m} + \boldsymbol{e}_r \frac{\hbar k}{m}\frac{|f(\theta)|^2}{r^2} \\
&+ \frac{\hbar\boldsymbol{k}}{2m}\frac{1}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}] \\
&+ \boldsymbol{e}_r \frac{\hbar k}{2mr}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}] \\
&+ \boldsymbol{e}_r \frac{i\hbar}{2mr^2}[f(\theta)e^{ikr(1-\cos\theta)} - f^*(\theta)e^{-ikr(1-\cos\theta)}] \\
&- \boldsymbol{e}_\theta \frac{i\hbar}{2mr^2}[\frac{\partial f(\theta)}{\partial\theta}e^{ikr(1-\cos\theta)} - \frac{\partial f^*(\theta)}{\partial\theta}e^{-ikr(1-\cos\theta)}] \\
&+ \boldsymbol{e}_\theta \frac{i\hbar}{2mr^2}[-\frac{\partial f(\theta)}{\partial\theta}f^*(\theta) + f(\theta)\frac{\partial f^*(\theta)}{\partial\theta}]
\end{aligned}
$$

For convenience, we define

$$\boldsymbol{J} = \boldsymbol{J}_1 + \boldsymbol{J}_2 + \boldsymbol{J}_3 + \boldsymbol{J}_4$$

to the order of $1/r$, with

$$\boldsymbol{J}_1 = \frac{\hbar\boldsymbol{k}}{m} = \frac{\hbar k}{m}(\boldsymbol{e}_r\cos\theta - \boldsymbol{e}_\theta\sin\theta),$$

$$\boldsymbol{J}_2 = \boldsymbol{e}_r \frac{\hbar k}{m}\frac{|f(\theta)|^2}{r^2}$$

$$\boldsymbol{J}_3 = \frac{\hbar\boldsymbol{k}}{2m}\frac{1}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$\boldsymbol{J}_4 = \boldsymbol{e}_r \frac{\hbar k}{2mr}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$\boldsymbol{J}_3 + \boldsymbol{J}_4 = \frac{\hbar \boldsymbol{k}}{2m}\frac{1}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$+\boldsymbol{e}_r \frac{\hbar k}{2mr}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$= \frac{\hbar k(\boldsymbol{e}_r \cos\theta - \boldsymbol{e}_\theta \sin\theta)}{2m}\frac{1}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$+\boldsymbol{e}_r \frac{\hbar k}{2mr}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$= \boldsymbol{e}_r \frac{\hbar k}{2m}\frac{(1+\cos\theta)}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$-\boldsymbol{e}_\theta \frac{\hbar k}{2mr}\frac{\sin\theta}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

We now consider the interference term which is defined by

$$\boldsymbol{J}_3 + \boldsymbol{J}_4 = \boldsymbol{e}_r \frac{\hbar k}{2m}\frac{(1+\cos\theta)}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

For $\theta \approx 0$,

$$\boldsymbol{J}_{\text{int}}(\boldsymbol{r}) = \boldsymbol{J}_3 + \boldsymbol{J}_4 == \boldsymbol{e}_r \frac{\hbar k}{m}\frac{1}{r}[f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

since $(1+\cos\theta)$ is smoothly changing function at $\theta = 0$.

(a) Contribution of $\boldsymbol{J}_3 + \boldsymbol{J}_4$ to the forward scattering

We now calculate the number of particles for the forward scattering for $0 \le \theta \le \delta\theta$

$$K = 2\pi r^2 \int_0^{\delta\theta} d\theta \sin\theta [\boldsymbol{J}_{\text{int}}(\boldsymbol{r}) \cdot \boldsymbol{e}_r]$$

$$= 2\pi r^2 \frac{\hbar k}{m}\frac{1}{r}\int_0^{\delta\theta} d\theta \sin\theta [f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$= \frac{2\pi\hbar kr}{m}\int_0^{\delta\theta} d\theta \sin\theta\, f(\theta)e^{ikr(1-\cos\theta)} + f^*(\theta)e^{-ikr(1-\cos\theta)}]$$

$$= \frac{2\pi\hbar kr}{m}\int_0^{\delta\theta} d\theta \sin\theta\, f(\theta)e^{ikr(1-\cos\theta)} + c.c.$$

where $\delta\theta$ is very small but is still finite. We assume that $f(\theta)$ has a sharp peak only at $\theta = 0$. Then the first term of K can be rewritten as

$$K = \frac{2\pi\hbar kr}{m}\int_0^{\pi} d\theta \sin\theta\, f(\theta) e^{ikr(1-\cos\theta)}$$

We set the following notation such that

$$x = kr, \qquad u = \cos\theta, \qquad h(u) = e^{ix(1-u)}, \qquad f(\theta) = F(u)$$

$$du = -\sin\theta d\theta$$

with

$$f(\theta = 0) = F(u = 1)$$

Then we have

$$K = \frac{2\pi\hbar}{m} x \int_{-1}^{1} du\, F(u) h(u) = \frac{2\pi\hbar}{m} x G(x)$$

with

$$G(x) = \int_{-1}^{1} du F(u) e^{ix(1-u)} = \int_{-1}^{1} du F(u) h(u)$$

We note that

$$\frac{i}{x}\frac{d}{du} e^{ix(1-u)} = e^{ix(1-u)}, \qquad \text{or} \qquad \frac{i}{x}\frac{dh(u)}{du} = h(u)$$

or

$$\left(\frac{i}{x}\right)^n \frac{d^n}{du^n} h(u) = h(u)$$

Now we calculate $G(x)$ for the two cases; $n = 2$ and $n = 3$.

(i) The choice of $n = 2$

$$G(x)=\int_{-1}^{1} duF(u)(\frac{i}{x})^2\frac{d^2h(u}{du^2})$$
$$=(\frac{i}{x})^2\int_{-1}^{1} duF(u)\frac{d^2h(u)}{du^2}$$
$$=(\frac{i}{x})^2\{[F(u)\frac{dh(u)}{du}]_{-1}^{1}-\int_{-1}^{1} du\frac{dF(u)}{du}\frac{dh(u)}{du}\}$$
$$=(\frac{i}{x})^2\{[F(u)\frac{dh(u)}{du}]_{-1}^{1}-[\frac{dF(u)}{du}h(u)]_{-1}^{1}+\int_{-1}^{1} du\frac{d^2F(u)}{d^2u}h(u)\}$$

This can be rewritten as

$$G(x)=(\frac{i}{x})^2\{[F(u)\frac{x}{i}h(u)]_{-1}^{1}-[\frac{dF(u)}{du}h(u)]_{-1}^{1}+\int_{-1}^{1} du\frac{d^2F(u)}{d^2u}h(u)\}$$
$$=\frac{i}{x}[F(u)h(u)]_{-1}^{1}-(\frac{i}{x})^2[\frac{dF(u)}{du}h(u)]_{-1}^{1}+(\frac{i}{x})^2\int_{-1}^{1} du\frac{d^2F(u)}{d^2u}h(u)$$

(ii) The choice of $n = 3$

$$G(x)=\int_{-1}^{1} duF(u)(\frac{i}{x})^3\frac{d^3h(u)}{du^3}$$
$$=(\frac{i}{x})^3\int_{-1}^{1} duF(u)\frac{d^3h(u)}{du^3}$$
$$=(\frac{i}{x})^3\{[F(u)\frac{d^2h(u)}{du^2}]_{-1}^{1}-\int_{-1}^{1} du\frac{dF(u)}{du}\frac{d^2h(u)}{du^2}\}$$
$$=(\frac{i}{x})^3\{[F(u)\frac{d^2h(u)}{du^2}]_{-1}^{1}-[\frac{dF(u)}{du}\frac{dh(u)}{du}]_{-1}^{1}+\int_{-1}^{1} du\frac{d^2F(u)}{du^2}\frac{dh(u)}{du}\}$$
$$=(\frac{i}{x})^3\{[F(u)\frac{d^2h(u)}{du^2}]_{-1}^{1}-[\frac{dF(u)}{du}\frac{dh(u)}{du}]_{-1}^{1}+[\frac{d^2F(u)}{du^2}h(u)]_{-1}^{1}-\int_{-1}^{1} du\frac{d^3F(u)}{du^3}h(u)\}$$

or

$$G(x)=(\frac{i}{x})[F(u)h(u)]_{-1}^{1}-(\frac{i}{x})^2[\frac{dF(u)}{du}h(u)]_{-1}^{1}$$
$$+(\frac{i}{x})^3[\frac{d^2F(u)}{du^2}h(u)]_{-1}^{1}-(\frac{i}{x})^3\int_{-1}^{1} du\frac{d^3F(u)}{du^3}h(u)\}$$

$F(u)$ is strongly localized about $u=1$ and is infinitely differentiable. We may thus assume that $F(u)$ and all of its derivatives at $u=-1$ vanish. In this case, $G_1(x)$ vanishes faster than any power of x.

$$\begin{aligned} G(x) &= (\frac{i}{x})[F(u)h(u)]_{-1}^{1} \\ &= \frac{i}{x}[F(1)h(1) - F(-1)h(-1)] \\ &= \frac{i}{x} f(0) \end{aligned}$$

in the limit of $x \to \infty$.

$$K = \frac{2\pi\hbar}{m} xG(x) + c.c. = \frac{2\pi\hbar}{m}[if(0) - if^*(0)] = -\frac{4\pi\hbar}{m}\mathrm{Im}[f(0)]$$

(b) The contribution of $\boldsymbol{J}_2 = \boldsymbol{e}_r \frac{\hbar k}{m}\frac{|f(0)|^2}{r^2}$ to the forward scattering

$$\begin{aligned} 2\pi r^2 \int_0^{\delta\theta} d\theta \sin\theta [J_2(\mathbf{r})\cdot \boldsymbol{e}_r] &= 2\pi r^2 \frac{\hbar k}{m}\int_0^{\delta\theta} d\theta \sin\theta \frac{|f(0)|^2}{r^2} \\ &= 2\pi \frac{\hbar k}{m} |f(0)|^2 \int_0^{\delta\theta} d\theta \sin\theta \\ &= 2\pi \frac{\hbar k}{m} |f(0)|^2 [1-\cos(\delta\theta)] \to 0 \end{aligned}$$

We note that

$$\boldsymbol{J}_1 = \frac{\hbar \boldsymbol{k}}{m} = \frac{\hbar k}{m}(\boldsymbol{e}_r \cos\theta - \boldsymbol{e}_\theta \sin\theta)$$

Then the contribution of $\mathbf{J}_1$ to the forward scattering is

$$\boldsymbol{J}_1 \cdot \boldsymbol{e}_r = \frac{\hbar k}{m}\cos\theta = \frac{\hbar k}{m}$$

So we have the contribution of the current density to the forward scattering is

$$\frac{\hbar k}{m} - \frac{4\pi\hbar}{m}\mathrm{Im}[f(0)]$$

7. The total scattering cross section (A. Das, lectures on Quantum mechanics)

For large r, we have

$$\psi^{(+)}(r,\theta) = \sum_l i^l \left(\frac{2l+1}{2ikr}\right)[e^{i2\delta_l} e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$
$$= \sum_l \left(\frac{2l+1}{2ikr}\right)[e^{i2\delta_l} e^{ikr} + (-1)^{l+1} e^{-ikr}]P_l(\cos\theta)$$

Here we rewrite

$$e^{i2\delta_l} \to S_l = \eta_l e^{i2\delta_l}$$

where η_l is real and $0 < \eta_l \leq 1$. We discuss later about the meaning of the parameter η_l. Then we have

$$\psi^{(+)}(r,\theta) = \sum_l \left(\frac{2l+1}{2ikr}\right)[S_l e^{ikr} + (-1)^{l+1} e^{-ikr}]P_l(\cos\theta)$$

The radial current probability density is

$$j_r = \frac{\hbar}{2mi}[\psi^{(+)^*}(r,\theta)\frac{\partial}{\partial r}\psi^{(+)}(r,\theta) - \frac{\partial}{\partial r}\psi^{(+)^*}(r,\theta)\,\psi^{(+)}(r,\theta)]$$

We note that

$$\psi^{(+)}(r,\theta) = \sum_l \left(\frac{2l+1}{2ikr}\right)[S_l e^{ikr} + (-1)^{l+1} e^{-ikr}]P_l(\cos\theta)$$

$$\frac{\partial}{\partial r}\psi^{(+)}(r,\theta) = \sum_l \left(\frac{2l+1}{2ikr}\right)[(ik)S_l e^{ikr} + (-1)^{l+1}(-ik)e^{-ikr}]P_l(\cos\theta)$$
$$= \sum_l \left(\frac{2l+1}{2r}\right)[S_l e^{ikr} - (-1)^{l+1} e^{-ikr}]P_l(\cos\theta)$$

$$\psi^{(+)^*}(r,\theta)\frac{\partial}{\partial r}\psi^{(+)}(r,\theta)-\frac{\partial}{\partial r}\psi^{(+)^*}(r,\theta)\,\psi^{(+)}(r,\theta)]$$

$$=-\sum_{l,l'}\left(\frac{2l+1}{2ikr}\right)\left(\frac{2l'+1}{2r}\right)[S_l^{*}e^{-ikr}+(-1)^{l+1}e^{ikr}][S_{l'}e^{ikr}-(-1)^{l'+1}e^{-ikr}]P_l(\cos\theta)P_{l'}(\cos\theta)$$

$$-\sum_{l,l'}\left(\frac{2l+1}{2r}\right)\left(\frac{2l'+1}{2ikr}\right)[S_l^{*}e^{-ikr}-(-1)^{l+1}e^{+ikr}][S_{l'}e^{ikr}+(-1)^{l'+1}e^{-ikr}]P_l(\cos\theta)P_{l'}(\cos\theta)]$$

$$=-\sum_{l,l'}\left(\frac{2l+1}{2ikr}\right)\left(\frac{2l'+1}{2r}\right)P_l(\cos\theta)P_{l'}(\cos\theta)$$

$$\times\{[S_l^{*}e^{-ikr}+(-1)^{l+1}e^{ikr}][S_{l'}e^{ikr}-(-1)^{l'+1}e^{-ikr}]+[S_l^{*}e^{-ikr}-(-1)^{l+1}e^{+ikr}][S_{l'}e^{ikr}+(-1)^{l'+1}e^{-ikr}]\}$$

$$=-\sum_{l,l'}\left(\frac{2l+1}{2ikr}\right)\left(\frac{2l'+1}{2r}\right)P_l(\cos\theta)P_{l'}(\cos\theta)$$

$$\times\{2S_l^{*}S_{l'}-(-1)^{l'+1}S_l^{*}e^{-2ikr}-(-1)^{l+1}e^{2ikr}S_{l'}-2(-1)^{l+l'}+(-1)^{l'+1}e^{-2ikr}S_l^{*}+(-1)^{l+1}e^{2ikr}S_{l'}\}$$

$$=\sum_{l,l'}\left(\frac{2l+1}{2ikr}\right)\left(\frac{2l'+1}{r}\right)P_l(\cos\theta)P_{l'}(\cos\theta)\times[-S_l^{*}S_{l'}+(-1)^{l+l'}]$$

At fixed $r=R$ (large sphere with a radius R), we have

$$\int da\, j_r = 2\pi R^2\int \sin\theta d\theta\; j_r$$

$$=\frac{\hbar}{2mi}2\pi R^2\sum_{l,l'}\left(\frac{2l+1}{2ikR}\right)\left(\frac{2l'+1}{R}\right)[-S_l^{*}S_{l'}+(-1)^{l+l'}]$$

$$\times\int_0^{\pi}P_l(\cos\theta)P_{l'}(\cos\theta)\sin\theta d\theta$$

$$=\frac{\hbar}{2mi}2\pi\sum_l\left(\frac{2l+1}{ik}\right)(1-|S_l|^2)$$

$$=\frac{\pi\hbar}{mk}\sum_{l=0}^{\infty}(2l+1)(|S_l|^2-1)$$

$$=\frac{\pi}{k^2}v\sum_{l=0}^{\infty}(2l+1)(|S_l|^2-1)$$

where v is the velocity of the incident particle and

$$\int_0^{\pi}\sin\theta d\theta\; P_l(\cos\theta)P_{l'}(\cos\theta)=\frac{2}{2l+1}\delta_{l,l'}$$

The scattering cross section for the inelastic scattering is obatined as

$$\sigma_{in} = -\frac{1}{v}\frac{\pi}{k^2}v\sum_{l=0}^{\infty}(2l+1)(|S_l|^2 - 1)$$
$$= -\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(|S_l|^2 - 1)$$
$$= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\eta_l{}^2)$$

When $|S_l| = \eta_l = 1$, the net flux moving out of a large sphere is zero. This is simply the conservation of probability. It states that the amount of particles that go in is the same as the number of particles that are scattered. However, there occur, in nature, processes in which the number of particles is not conserved in a scattering process. In fact, when a neutron is scattered off a complex nucleus, two things may happen. The neutron may scatter elastically. It may also scatter in-elastically by raising the nucleus to an excited state or may be absorbed by the nucleus. Clearly, this mean that the net radial flux out of a large sphere would not vanish in such cases. In fact, it should be negative since we are losing particles. Looking at the expression for the flux, it is clear that for this to happen, we need to have

$$|S_l|^2 < 1$$

8. Partial wave approximation for inelastic scattering

In the elastic scattering, we must have

$$S_l(k) = e^{2i\delta_l}$$

In the case where there is no flux loss, we must have $|S_l(k)| = 1$. However, this requirement is not valid whenever there is *absorption* of the incident beam. In this case, $S_l(k)$ is reduced by

$$S_l(k) = \eta_l(k)e^{2i\delta_l}$$

with

$$0 < \eta_l(k) \le 1.$$

Then we have

$$
\begin{aligned}
f_l(k) &= \frac{1}{2ik}[S_l(k)-1] \\
&= \frac{1}{2ik}[\eta_l(k)e^{2i\delta_l}-1] \\
&= \frac{1}{2k}[-i\eta_l(k)\{\cos(2\delta_l)+i\sin(2\delta_l)\}+i] \\
&= \frac{1}{2k}[\eta_l(k)\sin(2\delta_l)+i(1-\eta_l(k)\cos(2\delta_l))]
\end{aligned}
$$

The scattering amplitude is

$$
\begin{aligned}
f(\theta) &= \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)\frac{1}{i}[S_l(k)-1]P_l(\cos\theta) \\
&= \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)[\eta_l\sin(2\delta_l)+i(1-\eta_l\cos(2\delta_l))]P_l(\cos\theta)
\end{aligned}
$$

The scattering cross section for the elastic scattering is

$$
\begin{aligned}
\sigma_{el} &= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left|S_l-1\right|^2 \\
&= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[\eta_l^{\ 2}+1-2\eta_l\cos(2\delta_l)]
\end{aligned}
$$

Thus the total scattering cross section for the inelastic scattering can be evaluated as

$$
\begin{aligned}
\sigma_{tot} &= \sigma_{el}+\sigma_{in} \\
&= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[\eta_l^{\ 2}+1-2\eta_l\cos(2\delta_l)]+\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\eta_l^{\ 2}) \\
&= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\eta_l\cos(2\delta_l)]
\end{aligned}
$$

When $\eta_l \le 1$, $\sigma_{in} \ge 1$.

From the optical theorem with

$$
\operatorname{Im} f(\theta) = \sum_{l=0}^{\infty}\frac{2l+1}{2k}[1-\eta_l\cos(2\delta_l)]P_l(\cos\theta)
$$

so we get the total scattering cross section as

$$\sigma_{tot} = \frac{4\pi}{k}\mathrm{Im}[f(\theta = 0)]$$
$$= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\eta_l\cos(2\delta_l)]$$
$$= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\mathrm{Re}\,S_l)$$

This is in agreement with the expression of σ_{tot} obtained above.

((**Note**))

Since we do not specify what the inelastic processes consist of, we can only say about the total inelastic cross section, which describes the loss of flux.

Suppose that $\eta_l = 0$ we have the total absorption. Nevertheless there is still elastic scattering in that partial wave. This becomes evident in scattering by a black disc with a radius *a*. We consider the scattering for short wavelength, that is large *k*-values. The maximum value of *l* is $l_{\max} = ka$. Then we have the cross section of the inelastic scattering

$$\sigma_{in} = \frac{\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1) = \frac{\pi}{k^2}l_{\max}{}^2 = \pi a^2$$

and the cross section of the elastic scattering

$$\sigma_{el} = \frac{\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1) = \pi a^2$$

So the total cross section is

$$\sigma_{tot} = \sigma_{in} + \sigma_{el} = 2\pi a^2.$$

which is larger than πa^2, partly because of the shadow scattering (see Gasiorowiz).

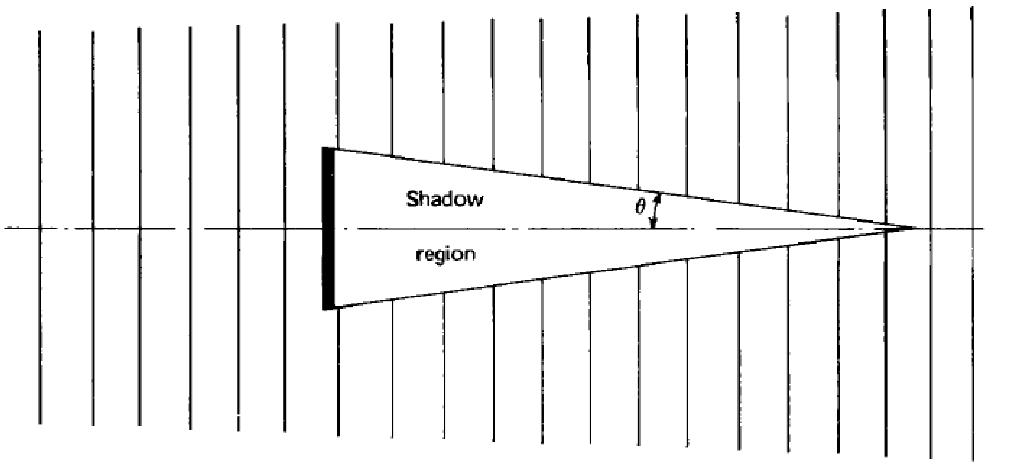


Fig. Black disc scattering and the shadow effect.

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9. The phase shift and the Green function

We use the following formula,

(i)

$$\frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} = 4\pi ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi'), \qquad (1)$$

where

$r_< = r$ for $r<r'$ and r' for $r'<r$.

$r_> = r$ for $r>r'$ and r' for $r'>r$.

and in the Cartesian co-ordinate,

$$\boldsymbol{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$\boldsymbol{r}' = (\sin\theta'\cos\phi', \sin\theta'\sin\phi', \cos\theta')$$

(ii)

$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr) , \tag{2}$$

(iii)

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}} \sum_l C_l (2l+1) i^l R_{kl}{}^{(+)}(r) P_l(\cos\theta) , \tag{3}$$

and

$$\psi^{(+)}(r,\theta) = \frac{1}{(2\pi)^{3/2}} e^{ikz} - \int d^3\mathbf{r}' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi |\mathbf{r}-\mathbf{r}'|} U(r') \psi^{(+)}(r',\theta') , \tag{4}$$

where

$$U(r) = \frac{2\mu}{\hbar^2} V(r) .$$

Using the above relations, we can derive the integral equation for $R_{kl}(r)$.

$$C_l R_{kl}{}^{(+)}(r) P_l(\cos\theta) = j_l(kr) P_l(\cos\theta)$$
$$- ikC_l \sum_{l'} \sum_{m'=-l'}^{l'} \int_0^{\infty} r'^2\, dr' j_{l'}(kr_<) h_{l'}^{(1)}(kr_>) U(r') R_{kl}{}^{(+)}(r') Y_{l'}^{m'}(\theta,\phi) \int_0^{\pi} \sin\theta' d\theta' \int_0^{2\pi} d\phi' Y_{l'}^{m'^*}(\theta',\phi') P_l(\cos\theta')$$

Here we note that

$$\begin{aligned}
\int_0^{\pi} \sin\theta' d\theta' \int_0^{2\pi} d\phi' Y_{l'}^{m'^*}(\theta',\phi') P_l(\cos\theta') &= 2\pi\delta_{m',0} \int_0^{\pi} \sin\theta' d\theta' Y_{l'}^{0^*}(\cos\theta') P_l(\cos\theta') \\
&= 2\pi\delta_{m',0} \sqrt{\frac{2l'+1}{4\pi}} \int_0^{\pi} \sin\theta' d\theta' P_{l'}(\cos\theta') P_l(\cos\theta') \\
&= 2\pi\delta_{m',0} \sqrt{\frac{2l'+1}{4\pi}} \frac{1}{2l'+1} 2\delta_{l,l'} \\
&= \sqrt{\frac{4\pi}{2l'+1}} \delta_{l,l'} \delta_{m',0} \\
&= \sqrt{\frac{4\pi}{2l+1}} \delta_{l,l'} \delta_{m',0}
\end{aligned}$$

where

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta),$$

$$\int_0^\pi \sin\theta d\theta P_{l'}(\cos\theta) P_l(\cos\theta) = \frac{2}{2l+1}\delta_{l,l'}.$$

Then we have

$$C_l R_{kl}{}^{(+)}(r) P_l(\cos\theta) = j_l(kr) P_l(\cos\theta)$$
$$-ikC_l \sum_{l'} \sum_{m'=-l'}^{l'} \delta_{l,l'}\delta_{m',0} \int_0^\infty r'^2\, dr' j_{l'}(kr_<) h_{l'}^{(1)}(kr_>) U(r') R_{kl}{}^{(+)}(r') \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \sqrt{\frac{4\pi}{2l+1}}$$

or

$$C_l R_{kl}{}^{(+)}(r) P_l(\cos\theta) = j_l(kr) P_l(\cos\theta)$$
$$-ikC_l \int_0^\infty r'^2\, dr' j_l(kr_<) h_l^{(1)}(kr_>) U(r') R_{kl}{}^{(+)}(r') P_l(\cos\theta)$$

or

$$C_l R_{kl}{}^{(+)}(r) = j_l(kr) - ikC_l \int_0^\infty r'^2\, dr' j_l(kr_<) h_l^{(1)}(kr_>) U(r') R_{kl}{}^{(+)}(r')$$

or

$$C_l R_{kl}{}^{(+)}(r) = j_l(kr) - ikC_l h_l^{(1)}(kr) \int_0^r r'^2\, dr' j_l(kr') U(r') R_{kl}{}^{(+)}(r')$$
$$-ikC_l j_l(kr) \int_r^\infty r'^2\, dr' h_l^{(1)}(kr') U(r') R_{kl}{}^{(+)}(r')$$

or

$$C_l R_{kl}{}^{(+)}(r) = j_l(kr) - ikC_l [j_l(kr) + in_l(kr)] \int_0^r r'^2\, dr' j_l(kr') U(r') R_{kl}{}^{(+)}(r')$$
$$-ikC_l j_l(kr) \int_r^\infty r'^2\, dr' [j_l(kr') + in_l(kr')] U(r') R_{kl}{}^{(+)}(r')$$

since

$$h_l^{(1)}(kr) = j_l(kr) + in_l(kr)\ .$$

Then we have

$$\begin{aligned}
C_l R_{kl}{}^{(+)}(r) = j_l(kr)[1 - ikC_l \int_0^r r'^2\, dr' j_l(kr')U(r')R_{kl}{}^{(+)}(r')] \\
+ kC_l \int_0^r r'^2\, dr' j_l(kr') n_l(kr) U(r') R_{kl}{}^{(+)}(r') \\
- ikC_l j_l(kr) \int_r^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}{}^{(+)}(r') \\
+ kC_l \int_r^\infty r'^2\, dr'\, j_l(kr) n_l(kr')] U(r') R_{kl}{}^{(+)}(r')
\end{aligned}$$

or

$$C_l R_{kl}{}^{(+)}(r) = j_l(kr)[1 - ikC_l \int_0^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}{}^{(+)}(r')]$$
$$+ kC_l \int_0^\infty r'^2\, dr' j_l(kr_<) n_l(kr_>) U(r') R_{kl}{}^{(+)}(r')$$

Here we choose C_l such that

$$C_l = 1 - ikC_l \int_0^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}{}^{(+)}(r')]$$

or

$$C_l = \frac{1}{1 + ik \int_0^\infty r'^2\, dr' j_l(kr')U(r')R_{kl}{}^{(+)}(r')]}$$

Then we get

$$R_{kl}{}^{(+)}(r) = j_l(kr) + k \int_0^\infty r'^2\, dr' j_l(kr_<) n_l(kr_>) U(r') R_{kl}{}^{(+)}(r')$$

10. Physical meaning of C_l and δ_l

We consider the physical meaning of C_l. For simplicity we assume that

$U(r) = 0$, for $r>a$.

We get

$$R_{kl}^{(+)}(r>a) = j_l(kr) + kn_l(kr)\int_0^r r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')$$

$$+kj_l(kr)\int_r^\infty r'^2\,dr' n_l(kr')U(r')R_{kl}^{(+)}(r')$$

$$= j_l(kr) + kn_l(kr)\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')$$

where we make use of our assumption that $U(r) = 0$ for $r>a$. The second term vanishes. The upper limit of integral in the first term extends from r to ∞.

If we choose

$$\tan\delta_l = -k\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r'), \tag{5}$$

then we get

$$R_{kl}^{(+)}(r>a) = j_l(kr) - \tan\delta_l n_l(kr)$$

$$= \frac{1}{\cos\delta_l}[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)] \tag{6}$$

and

$$C_l = \frac{1}{1+ik\int_0^\infty r'^2\,dr' j_l(kr')U(r')R_{kl}^{(+)}(r')]}$$

$$= \frac{1}{1-i\tan\delta_l} = e^{i\delta_l}\cos\delta_l$$

The wave function (for $r>a$) given by Eq.(3) has the form

$$\psi^{(+)}(r,\theta)=\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}e^{i\delta_l}(2l+1)i^l[\cos\delta_l j_l(kr)-\sin\delta_l n_l(kr)](r)P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}e^{i\delta_l}(2l+1)i^l[\left(\frac{e^{i\delta_l}+e^{-i\delta_l}}{2}\right)j_l(kr)-\left(\frac{e^{i\delta_l}-e^{-i\delta_l}}{2i}\right)n_l(kr)](r)P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}(\frac{2l+1}{2})i^l[e^{2i\delta_l}h_l^{(1)}(kr)+h_l^{(2)}(kr)](r)P_l(\cos\theta)$$

In the large limit of *r*, this solution is approximated by

$$\psi^{(+)}(r,\theta)=\frac{1}{(2\pi)^{3/2}}\sum_{l}(\frac{2l+1}{kr})i^l e^{i\delta_l}\sin(kr-\frac{l\pi}{2}+\delta_l)P_l(\cos\theta)$$

The asymptotic form of the incident plane wave is given by

$$e^{ikz}\to\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}\frac{i^l(2l+1)\sin(kr-\frac{l\pi}{2})}{kr}P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}i^l\left(\frac{2l+1}{2i}\right)\frac{1}{kr}[e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}]P_l(\cos\theta)$$

$$=\frac{1}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}\left(\frac{2l+1}{kr}\right)i^l\sin(kr-\frac{l\pi}{2})P_l(\cos\theta)$$

We note that the phase of the scattered wave shifts from that of the incident plane wave by the phase δ_l .

11. Born approximation from the phase shift

In the first Born approximation,

$$R_{kl}^{(+)}(r)\approx j_l(kr)$$

Then we have

$$\tan\delta_l^{(1)}\approx -k\int_0^{\infty}r'^2\,dr'[j_l(kr')]^2U(r')$$

This approximation is good when the phase shift is small. The function $j_l(kr)$ is approximated by

$$j_l(x)\approx\frac{2^l l!}{(2l+1)!}(x)^l .$$

Then we have

$$\tan\delta_l^{(1)} \approx -\frac{2^l (l!)^2}{[(2l+1)!]^2} k^{2l+1} \int_0^\infty r'^{2l+2}\, dr' U(r') .$$

For low energies and high angular momenta,

$$\delta_l^{(1)} \propto k^{2l+1} .$$

((**Example**)) The phase shift for l = 0 (s wave).

We assume that

$U(r) = -U_0$ for $r<a$, 0 for $r>a$.

Then we have

$$\tan\delta_l^{(1)} \approx -kU_0 \int_0^a r'^2\, dr' [j_0(kr')]^2$$
$$= \frac{U_0}{2k^2}[ak - \frac{\sin(2ak)}{2}]$$

When $ak << 1$, we get

$$\tan\delta_l^{(1)} \approx \delta_l^{(1)} = \frac{U_0 a^2}{3}(ak)$$

We note that $\delta_l^{(1)}$>0 for the attractive potential and $\delta_l^{(1)}$<0 for the repulsive potential.

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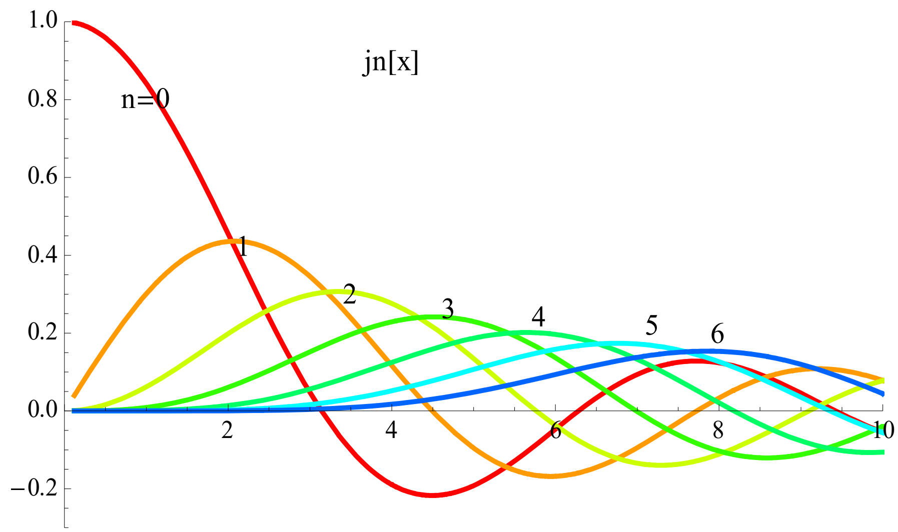
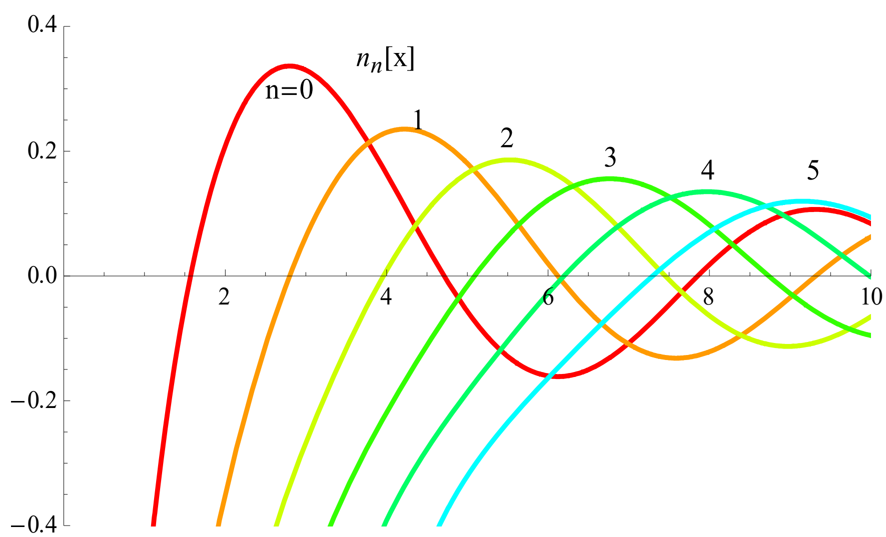
APPENDIX-I

((**Mathematica**))
Spherical Bessel function, spherical Neuman function, spherical Hankel function





APPENDIX-II Green function with spherical Bessel function

Free particle wave function ψ satisfies the Schrödinger equation

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

where m is the mass of particle, ($E_k = \frac{\hbar^2}{2m}k^2$) 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

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

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

(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

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

with

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

We put $x = kr$ (dimensionless)

$$\frac{\partial}{\partial r} = \frac{\partial x}{\partial r}\frac{\partial}{\partial x} = k\frac{\partial}{\partial x}, \qquad \frac{\partial^2}{\partial r^2} = k\frac{\partial}{\partial x}(k\frac{\partial}{\partial x}) = k^2\frac{\partial^2}{\partial x^2}$$

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

or

$$\frac{1}{x}\frac{d^2}{dx^2}(xR) + [1 - \frac{1}{x^2}\ell(\ell+1)]R = 0$$ (Spherical Bessel equation).

or

$$\frac{1}{x}[xR''+2R'] + [1 - \frac{1}{x^2}\ell(\ell+1)]R = 0$$

or

$$R'' + \frac{2}{x}R' + [1 - \frac{\ell(\ell+1)}{x^2}]R = 0$$

or

$$\frac{d}{dx}(x^2 R') + [x^2 - \ell(\ell+1)]R = 0.$$

This is a Sturm-Liouville-type differential equation.
Here we suppose that

$$R = \frac{J(x)}{\sqrt{x}},$$

$$\frac{d^2 J}{dx^2} + \frac{1}{x}\frac{dJ}{dx} + [1 - \frac{(\ell + \frac{1}{2})^2}{x^2}]J = 0.$$

The solution of this differential equation is

$$J(x) = J_{\ell+1/2}(x), \qquad \text{or} \qquad J(x) = N_{\ell+1/2}(x).$$

Then the solutions of R are obtained as the spherical Bessel functions defined by

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x),$$

and spherical Neumann function defined by

$$n_\ell(x) = \sqrt{\frac{\pi}{2x}} N_{\ell+1/2}(x).$$

Since the spherical Neumann function diverges at x =0, it cannot be chosen as a solution. Finally we have

$$\varphi_{k\ell m}(r,\theta,\phi) = \langle r,\theta,\phi | k,l,m \rangle = \sqrt{\frac{2k^2}{\pi}} j_\ell(kr) Y_{\ell m}(\theta,\phi),$$

with

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

and

$$\langle k'l'm' | klm \rangle = \delta(k-k')\delta_{l,l'}\delta_{m,m'}.$$

We define the spherical Hankel functions as

$$h_n^{(1)}(x) = \sqrt{\frac{\pi}{2x}} H^{(1)}_{n+\frac{1}{2}}(x) = j_n(x) + i n_n(x)$$

$$h_n^{(2)}(x) = \sqrt{\frac{\pi}{2x}} H^{(2)}_{n+\frac{1}{2}}(x) = j_n(x) - i n_n(x)$$

where the spherical Bessel function and spherical Neumann function are given by

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x)$$

$$n_n(x) = \sqrt{\frac{\pi}{2x}} N_{n+\frac{1}{2}}(x) = (-1)^n \sqrt{\frac{\pi}{2x}} J_{-n-\frac{1}{2}}(x)$$

Asymptotic forms

The asymptotic values of the spherical Bessel functions and spherical Hankel functions may be obtained from the Bessel asymptotic form.

$$j_\ell(x) \approx \frac{1}{x}\sin(x - \frac{l\pi}{2}),$$

$$n_\ell(x) \approx -\frac{1}{x}\cos(x - \frac{l\pi}{2}),$$

$$h_\ell^{(1)}(x) \approx -i\frac{e^{i(x-l\pi/2)}}{x} \qquad \text{(outgoing spherical wave)}$$

$$h_\ell^{(2)}(x) \approx i\frac{e^{-i(x-l\pi/2)}}{x} \qquad \text{(incoming spherical wave)}$$

Now we consider the Green's function given by

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

The solution of the Green's function is given by

$$G(\boldsymbol{r},\boldsymbol{r}') = \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}$$

with the boundary condition

$$G(\boldsymbol{r},\boldsymbol{r}') \to 0 \quad \text{for } r \to 0 \text{ and for } r \to \infty.$$

where $\boldsymbol{r}$ is the variable and $\boldsymbol{r}'$ is fixed.

Within each region (region I ($0<r<r'$) and region II ($r'<r$), we have the simpler equation

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

The solution of the Green's function is given by the form

$$G(\boldsymbol{r},\boldsymbol{r}') = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}(r,r',\theta',\phi')Y_l^m(\theta,\phi).$$

Then the differential equation of the Green's function is given by

$$\sum_{l',m'}[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'})+(k^2-\frac{l'(l'+1)}{r^2})A_{l'm'}]Y_{l'}^{m'}(\theta,\phi)=-\frac{\delta(r-r')}{r^2}\delta(\phi-\phi')\delta(\mu-\mu').$$

Note that

$$\delta_{l,l'}\delta_{m,m'}=\int d\Omega\langle l',m'|\mathbf{n}\rangle\langle\mathbf{n}|l,m\rangle=\iint\sin\theta d\theta d\phi Y_{l'}^{m'^*}(\theta,\phi)Y_l^m(\theta,\phi)$$

where

$$d\Omega=\sin\theta d\theta d\phi.$$

Then

$$\sum_{l',m'}\int d\Omega Y_l^{m^*}(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'.})+(k^2-\frac{l'(l'+1)}{r^2})A_{l'm'}]$$
$$=-\int d\Omega Y_l^{m^*}(\theta,\phi)\frac{\delta(r-r')}{r^2}\delta(\phi-\phi')\delta(\mu-\mu')$$

or

$$\sum_{l',m'}[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'})+(k^2-\frac{l'(l'+1)}{r^2})A_{l'm'}]\delta_{l,l'}\delta_{m,m'}$$
$$=-\int d\Omega Y_l^{m^*}(\theta,\phi)\frac{\delta(r-r')}{r^2}\delta(\phi-\phi')\delta(\mu-\mu')$$

or

$$\begin{aligned}\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{lm})+[k^2-\frac{l(l+1)}{r^2}]A_{lm}&=-\frac{\delta(r-r')}{r^2}\int d\Omega Y_l^{m^*}(\theta,\phi)\delta(\phi-\phi')\delta(\mu-\mu')\\&=-\frac{\delta(r-r')}{r^2}Y_l^{m^*}(\theta',\phi')\int d\mu d\phi\delta(\phi-\phi')\delta(\mu-\mu')\\&=-\frac{\delta(r-r')}{r^2}Y_l^{m^*}(\theta',\phi')\end{aligned}$$

Since $Y_l^{m^*}(\theta',\phi')$ is constant, we put

$$G_l(r,r')=\frac{A_{lm}(r,r',\theta',\phi')}{Y_l^{m^*}(\theta',\phi')}.$$

Then we get

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(rG_l)+[k^2-\frac{l(l+1)}{r^2}]G_l=-\frac{\delta(r-r')}{r^2},$$

The possible solutions of G_l are $j_l(kr)$, $n_l(kr)$, $h_l^{(1)}(kr)$, $h_l^{(1)}(kr)$, or a linear combination of these functions.

$G_{lI}=Aj_l(kr)$ for $r<r'$ (region I)

$G_{lII}=Bh_l^{(1)}(kr)$ for $r>r'$ (region II)

where A and B are constant. Note that If we use the positive sign for $G(\mathbf{r}, \mathbf{r}')$, we need to choose $h_l^{(1)}(kr)$;

$$h_\ell^{(1)}(kr)\approx -i\frac{e^{i(kr-l\pi/2)}}{kr}\approx\frac{e^{ikr}}{r}$$ (outgoing spherical wave)

(i) The continuity of G_l at $r = r'$

$$Aj_l(kr')=Bh_l^{(1)}(kr')$$

or

$$\frac{A}{h_l^{(1)}(kr')}=\frac{B}{j_l(kr')}=C$$

(ii) The discontinuity of dG_l/dr at $r = r'$.

$$\int_{r'-\varepsilon}^{r'+\varepsilon}\{\frac{d^2}{dr^2}(rG_l)+[k^2r-\frac{l(l+1)}{r}]G_l\}dr=-\int_{r'-\varepsilon}^{r'+\varepsilon}\frac{\delta(r-r')}{r}dr$$

or

$$[\frac{d}{dr}(rG_l)]_{r'-\varepsilon}^{r'+\varepsilon}=-\frac{1}{r'}$$

or

$$(G_l+r\frac{dG_l}{dr})|_{r'-\varepsilon}^{r'+\varepsilon}=-\frac{1}{r'}$$

$$\frac{dG_l^{II}(k,r,r')}{dr}|_{r'+\varepsilon}-\frac{dG_l^{I}(k,r,r')}{dr}|_{r'-\varepsilon}=-\frac{1}{r'^2}$$

or

$$kC[j_l(kr')h_l^{(1)}{}'(kr') - j_l{}'(kr')h_l^{(1)}(kr')] = -\frac{1}{r'^2}$$

We need to calculate the Wronskian

$$W = \begin{vmatrix} j_l(kr') & n_l(kr') \\ j_l{}'(kr') & n_l{}'(kr') \end{vmatrix} = \frac{i}{k^2 r'^2}$$

((**Mathematica**)) We can calculate *W* by using Mathematica.

```
Wronskian[{SphericalBesselJ[l, x],
  SphericalHankelH1[l, x]}, x]
```

$$\frac{i}{x^2}$$

Thus we get

$$C = ik$$

In general, we have

$$G(\mathbf{r},\mathbf{r}') = ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi')$$

.

This means that

$r_< = r$, $r_> = r'$ in the region I ($r<r'$)

$r_> = r$, $r_< = r'$ in the region II ($r'<r$)

We also get

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} = ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi')$$