Partial wave expansion and Geen's function

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(Date: April 23, 2015)

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)

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

with

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

where

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

and μ is a reduced mass. Note that $u_{kl}(r)$ 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

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

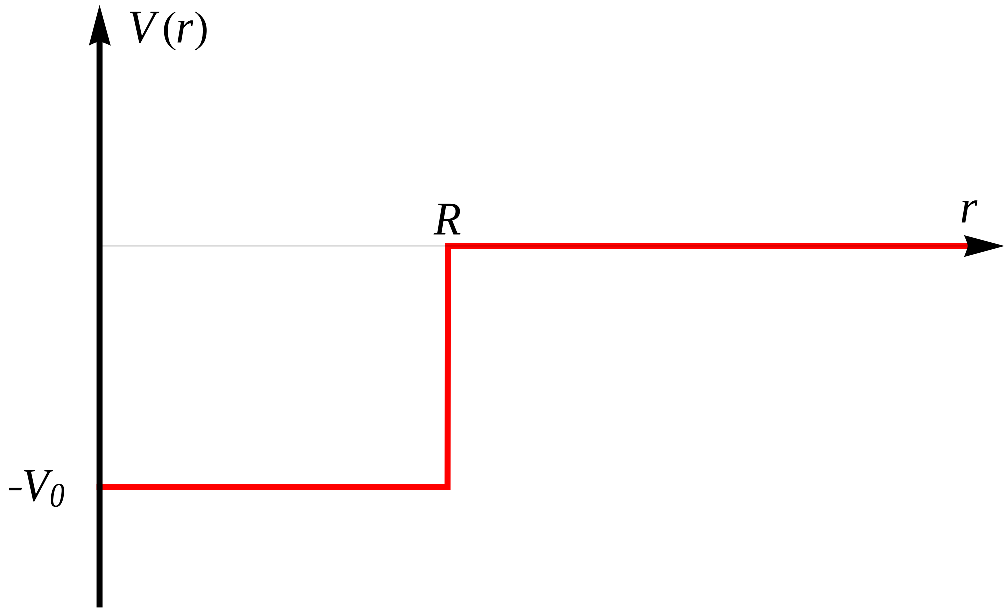


Fig. Attractive potential.

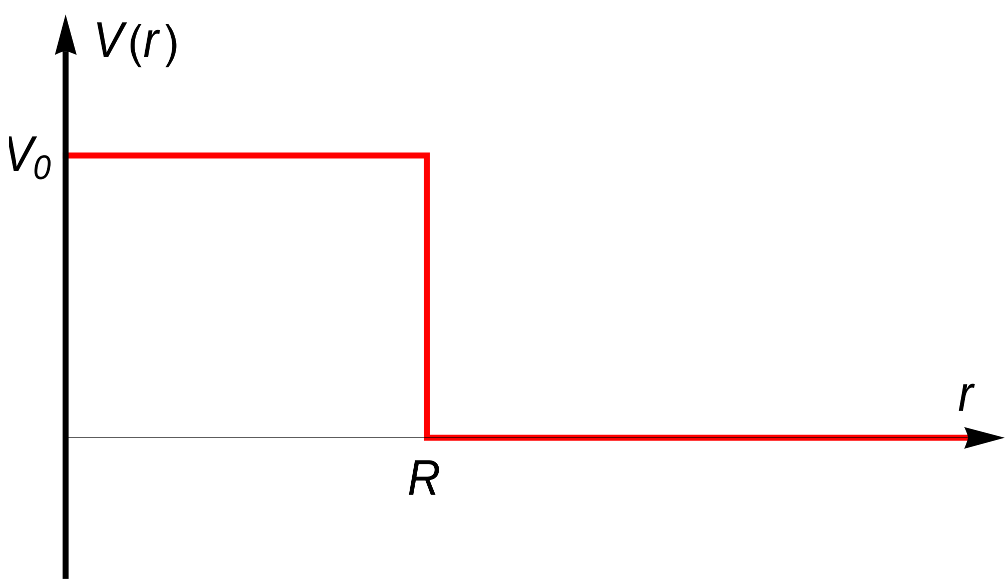


Fig. Repulsive potential

(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:

$$4\pi\gamma_l^{\ 2}\int_0^\infty drr^2[j_l(kr)]^2 = 1$$

2. Semiclassical argument for the angular momentum,

((Classical mechanics))

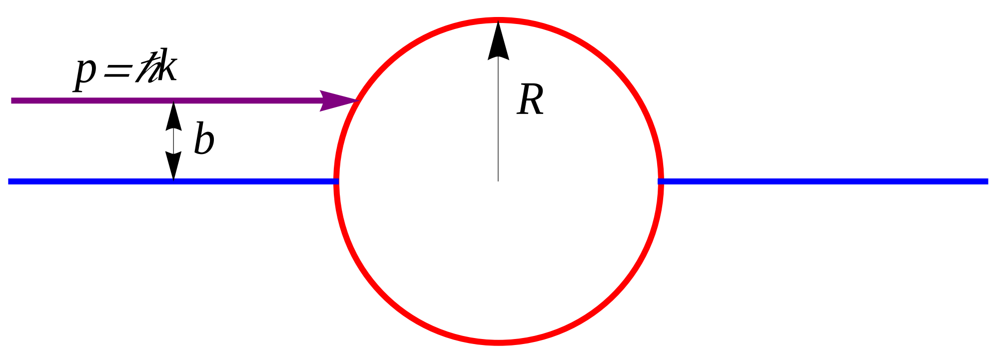
The particles with the impact parameter b possesses the angular momentum L given by

$$L = pb\,,$$

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

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

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

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

$$= a_l \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr}$$

or

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

If the potential is spherically symmetric, the scattering amplitude $\psi^{(+)}(r,\theta)$ is a function of r and θ:

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

($m = 0$), leading to the form

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

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

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

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

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

where the replacement of the coefficient is made as

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

((**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)

Since

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

we get

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

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),

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

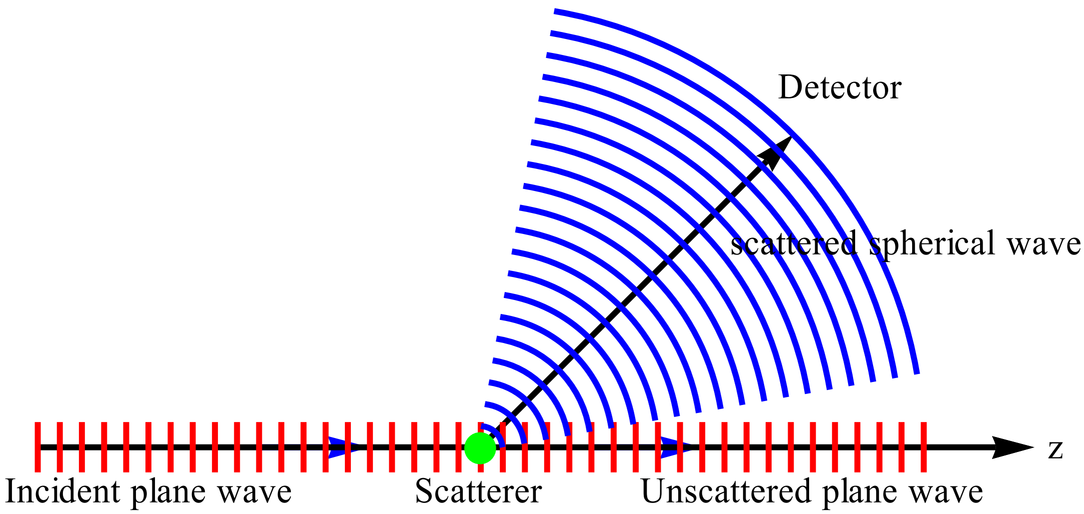


Fig. Schematic layout for scattering experiment. The scattering angle is the laboratory angle.

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 comparison leads to the condition for a_l.

$$-a_l e^{-i\delta_l} + 1 = 0, \qquad \text{or} \qquad a_l = e^{i\delta_l}.$$

from the coefficient of $e^{-i(kr-\frac{l\pi}{2})}$. Then

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

Noting that

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

we have

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

with

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

or

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

$f_l(k)$ 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 Schrodinger'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

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

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 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 [$(\hbar k/m)\sigma_{tot}$].

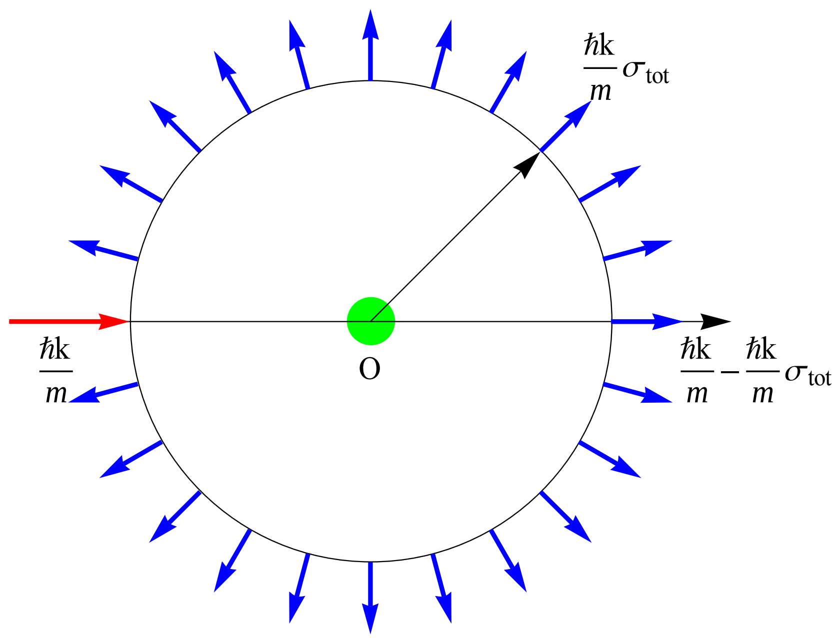


Fig. **Optical theorem**. The intensity of the incident wave is $\hbar k/m$. The intensity of the forward wave is $(\hbar k/m)-(4\pi\hbar/m)\,\mathrm{Im}[f(0)]$. The waves with the total intensity $(4\pi\hbar/m)\,\mathrm{Im}[f(0)]=(\hbar k/m)\sigma_{tot}$ is scattered for all the directions, as the scattering 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 ½ centered at (i/2).

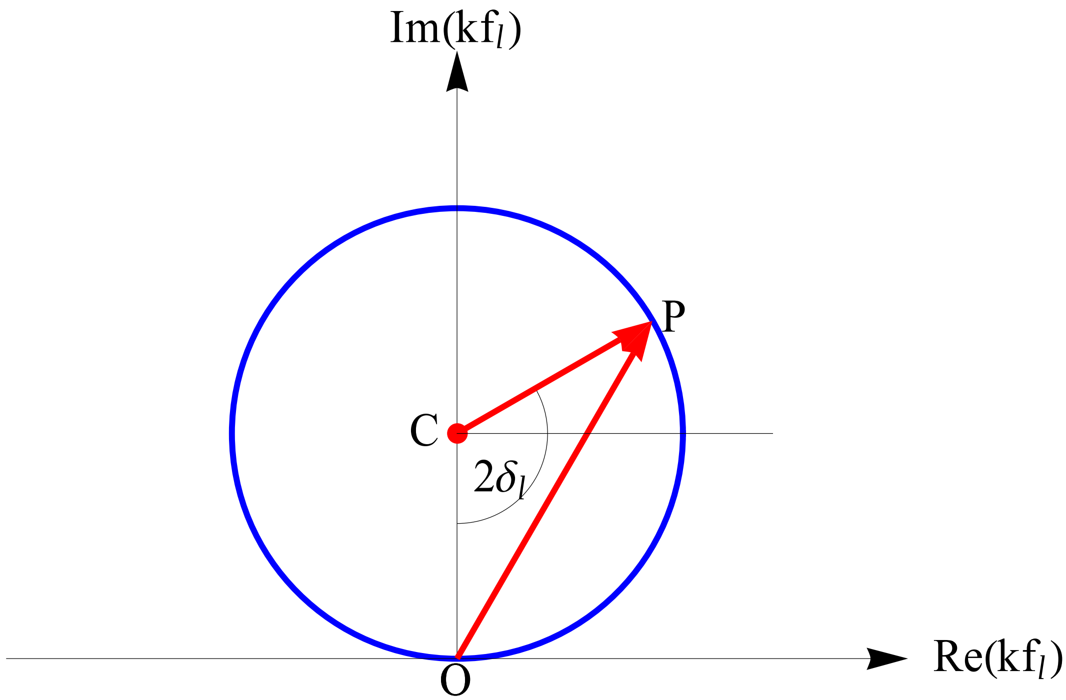


Fig. Argand diagram of $z = kf_l(k)$; The circle is called the *unitary circle*.

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

(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. Partial wave approximation for inelastic scattering

In the elastic scattering, we must have

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

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

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

The total elastic scattering cross section is given by

$$\sigma_{el} = 4\pi\sum_{l=0}^{\infty}(2l+1)\left|f_l(k)\right|^2 = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1+\eta_l^{\,2} - 2\eta_l \cos(2\delta_l)]$$

The total inelastic scattering cross section is

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

The total cross section is

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

7. The phase shift and the Green function

We use the following formula,

(i)

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

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

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

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

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

$$+ kC_l \int_0^r r'^2\, dr' j_l(kr')n_l(kr)U(r')R_{kl}^{(+)}(r')$$

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

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

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

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

7. 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

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

then we get

$$R_{kl}^{(+)}(r>a) = j_l(kr) - \tan\delta_l n_l(kr)$$
$$= \frac{1}{\cos\delta_l}[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)] \qquad (6)$$

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

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

The asymptotic form of the incident plane wave is given by

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

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

8. Born approximation from the phase shift

In the first Born approximation,

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

Then we have

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

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

$$U(r) = -U_0 \quad \text{for } r<a, \text{ 0 for } r>a.$$

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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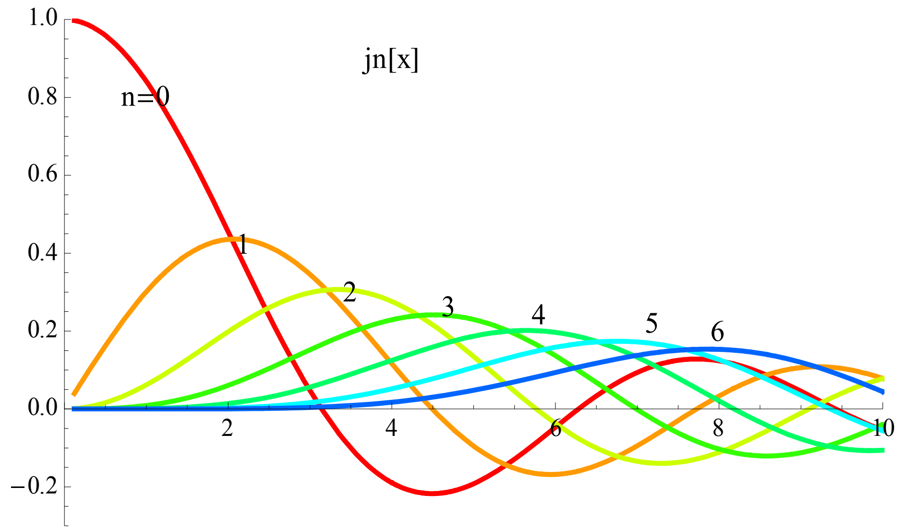
APPENDIX

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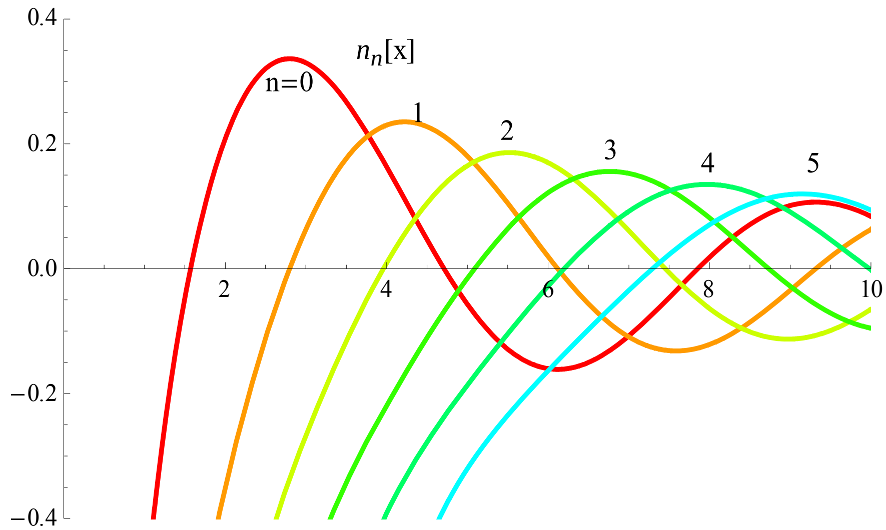
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