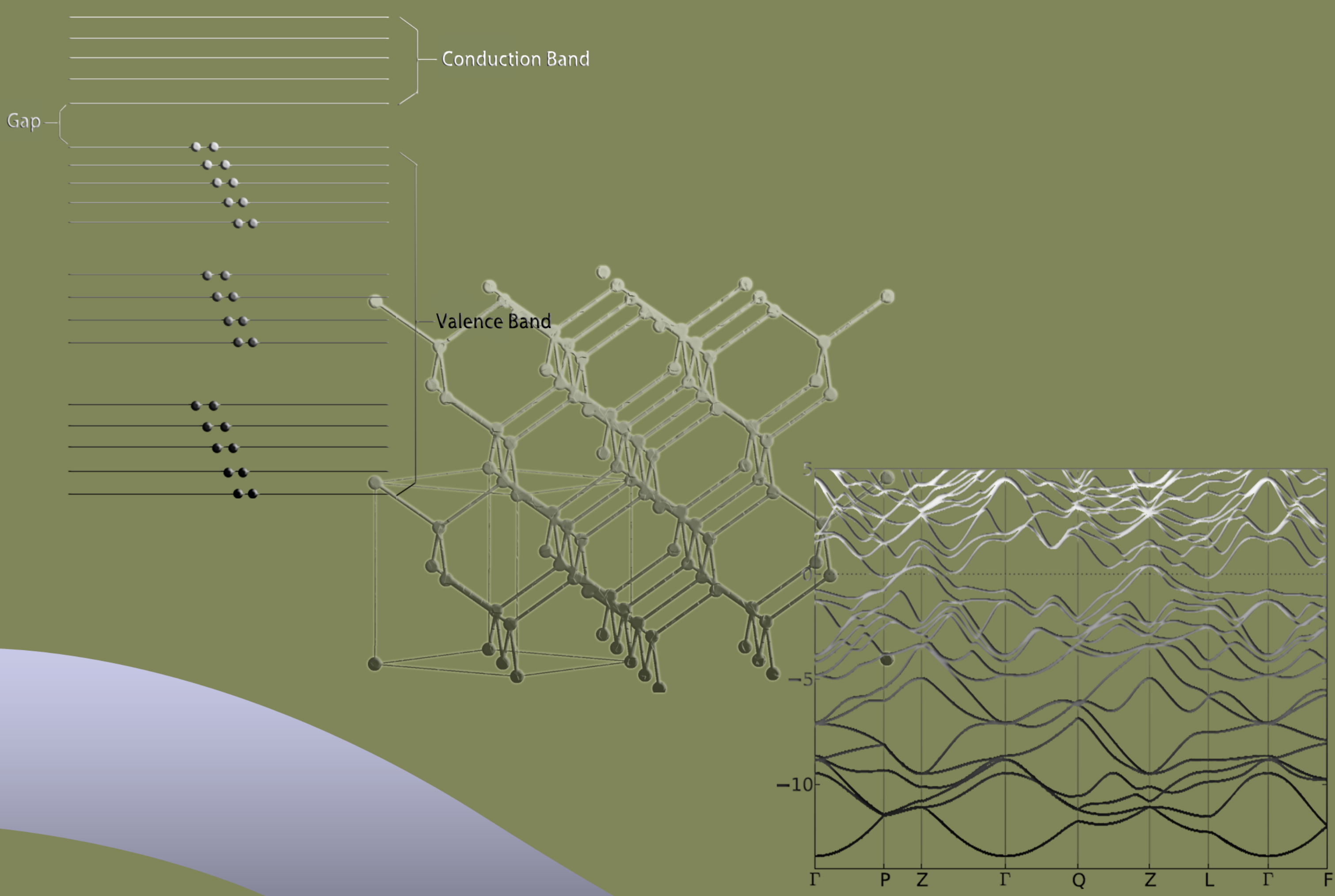
Queen Mary, University of London

School of Physics and Astronomy

Quantum scattering theory basics



1. What is scattering?

Classically, when talking about scattering, we often refer the collision between one particle with another (or can be particle system). Briefly, if we think about two balls' interaction, the scattering process can be described as the collision between the two balls, and then the definition of *scattering cross section* is natural: how large the interaction area is. Now if we fix one of the balls and focus on the other one, if the energy of the scattered ball is kept after scattering process (collision), we say this kind of scattering is *elastic*. Accordingly, we can imagine *inelastic scattering* if the energy of scattered ball is changed.

When coming to quantum field, the scattering process cannot be described simply as collision. The 'ball' here becomes wave-function, and there should be another system which the incoming wave-function interacts with — a potential field where the incident wave-function is propagating. Hence the scattering in quantum field refers to the influence of external potential field upon the incident wave-function. Again, we have definition for *cross section*, which does not mean the real interaction area but the probability of incoming wave being scattered. If only the momentum of incoming wave is changed after scattering, it is called *elastic scattering*, and *inelastic* for energy loss case.

For the convenience of following discussion, there should be more about *cross section*, *elastic* and *inelastic scattering* to introduce. First the *cross section*: if we assume the incident beam is plane and the outgoing scattered wave becomes spherical wave centering at the scattering point, the *cross section* then defines how much of the plane wave is destructed and changed to spherical wave. As for how the plane wave is destructed, it will be discussed in details in following part. And the *inelastic scattering* here in this case means there is flux loss of the outgoing spherical wave.

2. Phase shift and wave amplitude

Assuming the incident wave is along z-axis:

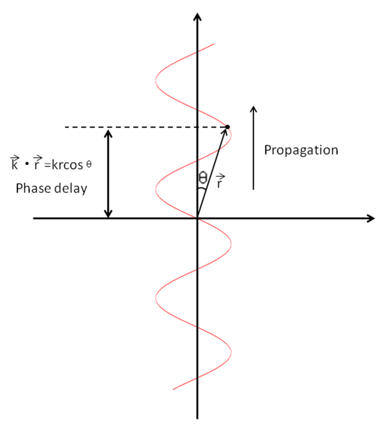


Figure 1. Incident wave prorogating along z-axis.

Here also it is assumed that the incoming beam is plane wave (For details about plane wave, refer to Appendix-1), and the wave-function can be written as:

$$\phi_{inc}(\vec{r}) = exp(i\vec{k}\cdot\vec{r}) = exp(ikrcos\theta) \tag{2-1}$$

Then express the plane wave in terms of superposition angular momentum eigenstates:

$$exp(i\vec{k}\cdot\vec{r}) = \sum_{l=0}^{\infty} i^l(2l+1)j_l(kr)P_l(cos\theta) \tag{2-2}$$

Actually, it is the expression of plane wave as a sum of spherical waves (details refer to corresponding Wikipage). Therefore each component can be examined about how to be distorted by the external potential, and this method is thus called *partial wave analysis*.
Now assuming the external potential is spherically symmetric, which keeps the angular momentum of incident wave conserved, the corresponding Schrödinger equation can be given as:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \tag{2-3}$$

By splitting variables to radius-concerned-only and angle-concerned-only, and expressing the equation in spherical coordinate, the solution for equation - 2-3 can be written as (details refer to Schrödinger Equation in Spherical Coordinates):

$$\psi(r,\theta) = \sum_{l=0}^{\infty} a_l R_{kl}(r)P_l(cos\theta) \tag{2-4}$$

Here we have: $k^2 = \frac{2mE}{\hbar^2}$, and $P_l(cos\theta)$ is Legendre Polynomial and $R_{kl}(r)$ obeys:

$$[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}][rR_{kl}(r)] = \frac{2m}{r^2}V(r)[rR_{kl}(r)] \tag{2-5}$$

2-4 is just the direct result of scattering effect potential $V(\vec{r})$ by solving corresponding Schrödinger equation - 2-3.
There is another way to express scattering result:

$$\begin{aligned}\psi(\vec{r}) &= \phi_{inc}(\vec{r}) + \phi_{sc}(\vec{r}) \\ &= A[e^{i\vec{k}_0\cdot\vec{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}]\end{aligned} \tag{2-6}$$

which means the scattered wave is the combination of incident plane wave and the resulting spherical wave (by scattering, part of the plane wave changes to spherical wave), and $f(\theta,\phi)$ describes how much plane wave was changed to spherical form (scattered). The process can be depicted in Fig. 2. If assuming the external potential is spherically symmetric, the scattered spherical wave should be also central symmetric, which then makes the scattering result nothing to do with azimuthal angle

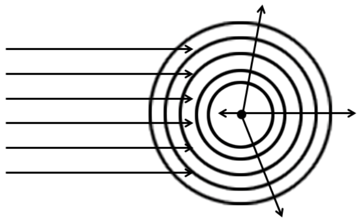


Figure 2. Incident plane wave and scattered spherical wave illustration.

ϕ. Furthermore, assuming elastic scattering (then $\vec{k}_0 = \vec{k}$) and considering plane wave expansion 2-2, 2-6 can be written as:

$$\psi(r,\theta) = \sum_{l=0}^{\infty} i^l(2l+1)j_l(kl)P_l(cos\theta) + f(\theta)\frac{e^{ikr}}{r} \tag{2-7}$$

Since the real detection always locate the detector far away from the target (compared to the size of target itself), we then have the limit condition: $r \to \infty$. In this limit, we have:

$$\lim_{r\to\infty} j_l(kl) = \frac{sin(kr - \frac{l\pi}{2})}{r} \tag{2-8}$$

Then we have:

$$sin(kr - \frac{l\pi}{2}) = \frac{(-i)^l e^{ikr} - i^l e^{-ikr}}{2i} \tag{2-9}$$

by using:

$$e^{\pm\frac{il\pi}{2}} = (e^{\pm\frac{i\pi}{2}})^l = (\pm i)^l \tag{2-10}$$

So:

$$\begin{aligned}
\lim_{r\to\infty}\psi(r,\theta) &= \sum_{l=0}^{\infty} i^l(2l+1)P_l(cos\theta)\frac{sin(kr-\frac{l\pi}{2})}{kr} + f(\theta)\frac{e^{ikr}}{r} \\
&= \sum_{l=0}^{\infty} i^l(2l+1)P_l(cos\theta)[\frac{(-i)^l e^{ikr} - i^l e^{-ikr}}{2ikr}] + f(\theta)\frac{e^{ikr}}{r} \\
&= -\frac{i^l e^{-ikr}}{2ikr}\sum_{l=0}^{\infty} i^l(2l+1)P_l(cos\theta) + \sum_{l=0}^{\infty}\frac{(-i)^l e^{ikr}}{2ikr} i^l(2l+1)P_l(cos\theta) + f(\theta)\frac{e^{ikr}}{r} \\
&= -\frac{e^{-ikr}}{2ikr}\sum_{l=0}^{\infty} i^{2l}(2l+1)P_l(cos\theta) + \frac{e^{ikr}}{r}[f(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty} i^l(-i)^l(2l+1)P_l(cos\theta)]
\end{aligned} \tag{2-11}$$

2-11 is the asymptotic form ($r \to \infty$) of final scattering result.

Recalling we have already obtained the scattered wave-function directly by solving Schrödinger equation:

$$\psi(r,\theta) = \sum_{l=0}^{\infty} a_l R_{kl}(r)P_l(cos\theta) \tag{2-12}$$

And again, we need to find the asymptotic form of 2-12 when $r \to \infty$. Starting from 2-5, and considering the effective scattering potential should be 0 when $r \to \infty$, 2-5 then becomes:

$$(\frac{d^2}{dr^2} + k^2)[rR_{kl}(r)] = 0 \tag{2-13}$$

2-13 is the standard Helmholtz Equation, for which the solution is given by a linear combination of the spherical Bessel and Neumann (also known as Bessel functions of the second kind) functions:

$$R_{kl}(r) = A_l j_l(kr) + B_l \eta_l(kr) \tag{2-14}$$

$r \to \infty$ gives:

$$\lim_{r\to\infty} \eta_l(kr) = -\frac{cos(kr - \frac{l\pi}{2})}{kr} \tag{2-15}$$

Then 2-8 and 2-15 togethers gives:

$$\lim_{r\to\infty} R_{kl}(r) = A_l \frac{sin(kr - \frac{l\pi}{2})}{kr} - B_l \frac{cos(kr - \frac{l\pi}{2})}{kr} \tag{2-16}$$

Here the coefficient A_l and B_l is independent, and 2-16 stands for all $V(r)$ form. So if we have $V(r) = 0$, which refers to free particle, for $r \to 0$ we should have:

$$\lim_{r\to 0} rR_{kl}(r) = 0 \tag{2-17}$$

$$\Rightarrow$$

$$R_{kl}(r) \to finite$$

However if A_l and B_l is independent as stated before, the divergence of 2-16 either first or second term will then make the solution 2-16 non-physical. Hence we should arbitrarily introduce relationship between A_l and B_l, and here we rewrite 2-16 as:

$$R_{kl}(r) = C_l[cos(\delta_l)j_l(kr) - sin(\delta_l)\eta_l(kr)] \tag{2-18}$$

where:

$$\begin{aligned} &A_l = C_l cos(\delta_l), \quad B_l = C_l sin(\delta_l) \\ &\delta_l = -tan^{-1}(\frac{B_l}{A_l}) \end{aligned} \tag{2-19}$$

Then we have:

$$\begin{aligned} \lim_{r\to\infty} R_{kl}(r) &= C_l \frac{cos(\delta_l)sin(kr - \frac{l\pi}{2}) - sin(\delta_l)cos(kr - \frac{l\pi}{2})}{kr} \\ &= C_l \frac{sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \end{aligned} \tag{2-20}$$

Here if we have $V(r) = 0$ for all r (no external potential, hence no scattering everywhere), we should have $\delta_l = 0$. In all the other cases, $\delta_l \neq 0$ which means there is a *phase shift* due to the existence of external potential $V(r)$. Here it should be noticed that the form of potential determines corresponding phase shift δ_l, which should also be adjusted for each l component.
The solution for scattering form 2-4 then becomes:

$$\lim_{r\to\infty} \psi(r,\theta) = \sum_{l=0}^{\infty} a_l P_l(cos\theta) \frac{sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \tag{2-21}$$

since:

$$sin(kr - \frac{l\pi}{2} + \delta_l) = \frac{(-i)^l e^{ikr} e^{i\delta_l} - i^l e^{-ikr} e^{-i\delta_l}}{2i} \tag{2-22}$$

2-21 then becomes:

$$\lim_{r\to\infty} \psi(r,\theta) = -\frac{e^{-ikr}}{2ikr}\sum_{l=0}^{\infty} a_l i^l e^{-i\delta_l} P_l(cos\theta) + \frac{e^{ikr}}{2ikr}\sum_{l=0}^{\infty} a_l (-i)^l e^{i\delta_l} P_l(cos\theta) \tag{2-23}$$

Recalling the asymptotic form of scattering wave 2-11 and compare with the asymptotic form of direction solution for corresponding scattering Schrödinger equation 2-23, we can obtain following relationships:

$$a_l i^l e^{-i\delta_l} = i^{2l}(2l+1) \tag{2-24}$$

$$f(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty} i^l(-i)^l(2l+1)P_l(cos\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty} a_l(-i)^l e^{i\delta_l} P_l(cos\theta) \tag{2-25}$$

According to 2-24:

$$a_l = (2l+1)i^l e^{i\delta_l} \tag{2-26}$$

Substituting 2-26 into 2-25:

$$f(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty} i^l(-i)^l(2l+1)P_l(cos\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)i^l(-i)^l e^{i\delta_l} e^{i\delta_l} P_l(cos\theta) \tag{2-27}$$

Since $i^l(-i)^l = 1$:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2ik} - 1)P_l(cos\theta) \tag{2-28}$$

By using the following relation:

$$\frac{e^{2ik} - 1}{2i} = e^{i\delta_l} sin(\delta_l) \tag{2-29}$$

2-28 becomes:

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l} sin(\delta_l) P_l(cos\theta) \tag{2-30}$$

$$= \sum_{l=0}^{\infty} f_l(\theta) \tag{2-31}$$

Thereby, we obtain the expression for $f(\theta)$ which describes how the incident plane wave is changed to the scattering spherical wave. And $f_l(\theta)$ here is given the name of *partial wave amplitude*. Furthermore, we should have the definition for *differential cross section*, which is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)(2l'+1)e^{i(\delta_l - \delta_{l'})} sin(\delta_l) sin(\delta_{l'}) P_l(cos\theta) P_{l'}(cos\theta) \tag{2-32}$$

Then the *total cross section* is:

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{\pi} |f(\theta)|^2 sin\theta d\theta \int_0^{2\pi} d\phi$$
$$= 2\pi \int_0^{\pi} |f(\theta)|^2 sin\theta d\theta \tag{2-33}$$

Considering 2-32, we have:

$$\sigma = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (2l+1)(2l'+1) e^{i(\delta_l - \delta_{l'})} sin(\delta_l) sin(\delta_{l'}) \int_0^{\pi} P_l(cos\theta) P_{l'}(cos\theta) sin\theta d\theta \tag{2-34}$$

Also we have:

$$\int_0^{\pi} P_l(cos\theta) P_{l'}(cos\theta) sin\theta d\theta = \frac{2}{2l+1} \delta_{ll'} \tag{2-35}$$

So:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{4\pi} (2l+1) sin^2(\delta_l)$$
$$= \sum_{l=0}^{\infty} \sigma_l \tag{2-36}$$

By writing as the sum form, we can separate the *total cross section* to *partial cross section*, describing the scattering of each angular momentum component.

3. Optical Theorem

For 2-30, there is a special case when $\theta = 0$, where we have:

$$f(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)[sin(\delta_l) cos(\delta_l) + i sin^2(\delta_l)] \tag{3-1}$$

Then we can establish the following relation:

$$\frac{4\pi}{k} Im f(0) = \sigma = \frac{4\pi}{k} \sum_{l=0}^{\infty} (2l+1) sin^2(\delta_l) \tag{3-2}$$

This is the so-called *Optical Theorem*, which links the loss of incident beam (*total cross section* — σ) with the created spherical scattering wave at ($\theta = 0$) — $f(0)$. The physical origin can be described as: Scattering is the process of incident plane wave removal to become spherical wave. Then how is the plane wave removed? From physical viewpoint, the removal can only come from the destructive interference of scattering spherical wave with incoming plane wave. However only when $\theta = 0$ does the scattering spherical wave propagates along the same direction with the incident plane wave. That's why we can establish the link between *total cross section* — σ with *total wave amplitude* at ($\theta = 0$) — $f(0)$.

4. Inelastic Scattering

After scattering, the plane wave changes to spherical wave by factor $f(\theta)$. The scattering process accompanies the flux loss of incident plane wave as stated before. However in real case, there should be also flux loss for outgoing spherical wave, and this part of flux loss is called *inelastic scattering* effect.

Recalling 2-11, the first term in 2-11 contains 'e^{-ikr}/r' which refers to the inwards spherical wave, and the second term contains 'e^{ikr}/r' which represents outwards wave. When we talk about the flux loss of outgoing spherical wave after scattering, we actually refer to the second term which is in fact what is finally 'seen' by the detector (because it is 'outwards' as is said at the beginning). Considering 2-11 and 2-27 at the same time, if we are to introduce flux loss factor, it should be the right side of 2-27 where this flux loss factor $\eta_l(k)$ should be added. Then if we define:

$$S_l(k) = e^{2i\delta_l}, \quad no\ flux\ loss \tag{4-1}$$

$$S_l(k) = \eta_l(k)e^{2i\delta_l}, \quad flus\ loss \tag{4-2}$$

Then for flux loss case, 2-27 can be rewritten as:

$$\begin{aligned}
f(\theta) &= \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[S_l(k)-1]P_l(cos\theta) \\
&= \sum_{l=0}^{\infty}(2l+1)\frac{\eta_l(k)e^{2i\delta_l}-1}{2ik}P_l(cos\theta) \\
&= \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)\frac{\eta_l(k)[cos(2\delta_l)+isin(2\delta_l)]-1}{i}P_l(cos\theta) \\
&= \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)\{\eta_l(k)sin(2\delta_l)+i[1-\eta_l(k)cos(2\delta_l)]\}P_l(cos\theta)
\end{aligned} \tag{4-3}$$

To obtain the *total elastic cross section*, we need to do integration for modulus square of 4-3 upon θ (the same route given by 2-33). Again considering 2-35, we have:

$$\begin{aligned}
\sigma_{el} &= 4\pi\sum_{l=0}^{\infty}(2l+1)[\frac{\eta_l(k)sin(2\delta_l)+i[1-\eta_l(k)cos(2\delta_l)]}{2k}]^2 \\
&= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1+\eta_l^2(k)-2\eta_l(k)cos(2\delta_l)]
\end{aligned} \tag{4-4}$$

Then considering the introduction of flux loss factor $\eta_l(k)$ given in 4-2 and the whole outgoing spherical wave (right side of 2-27), the *total inelastic scattering cross section* (the flux loss) can be given by:

$$\sigma_{inel} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\eta_l^2(k)] \tag{4-5}$$

The *total cross section* when there is *inelastic scattering* can be given as:

$$\begin{aligned}\sigma_{tot} &= \sigma_{el} + \sigma_{inel} \\ &= \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\eta_l(k)cos(2\delta_l)]\end{aligned} \tag{4-6}$$

Recalling 4-3, we have:

$$Imf(0) = \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)[1-\eta_l(k)cos(2\delta_l)] \tag{4-7}$$

By comparing 4-6 with 4-7:

$$Imf(0) = \frac{k}{4\pi}\sigma_{tot} \tag{4-8}$$

which means the *Optical Theorem* also stands for *inelastic scattering*.

Then we go back to 2-27, 2-28 and 4-2, it should be noticed the difference between $f(\theta)$ and the introduced flux loss factor $\eta_l(k)$. Both of them refers to *flux loss*, while $f(\theta)$ means the flux loss of incident plane wave which then transforms to scattered spherical wave, however $\eta_l(k)$ means the flux loss of outgoing spherical wave which then contribute to the *inelastic scattering*.

Appendices

1. Plane Wave

The following is the illustration of plane wave:

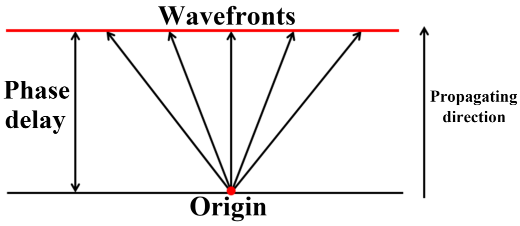


Figure 3. Wavefronts of plane wave.

The common mathematics form of wave equation is:

$$\nabla^2 f - \frac{1}{v^2}\frac{\partial^2 f}{\partial t^2} = 0 \tag{A1-1}$$

Here, $f(x,t)$ is the wave function, and v is the prorogation speed of the wave. x is the position and t is time. The wave equation - A1-1 can be derived in many ways as stated on Wikipage. Also the Wikipage gives one of the derivations based on Hooke's law, from which details about derivation process can be found. There is one key point to clear — 'v' within equation - A1-1, which we assign as the propagation velocity of the wave. The reason for this can only be seen after the solution form of equation - A1-1 is given.

How can we get the solution? Actually, the wave is the propagation of vibration, and the vibration at one point can be described by cos function as: $cos(\omega t + \phi)$, where ω is the angular frequency of the vibration. Then if we say the wave propagates along x-axis, there should be phase delay along x-axis — the vibration of point far from origin starts later than that near the origin. Then how much is the delay at point x? If recalling the definition of wave number $k = \frac{2\pi}{\lambda}$, it is actually gives the phase delay 'unit' (If propagating one unit in space, the phase delay is just $\frac{2\pi}{\lambda}$. If propagating λ — one wavelength in space, the phase delay is just 2π — equivalent one period in time). Hence the phase delay at point x can be easily given as: kx. Thereby we can establish the common solution for equation - A1-1:

$$f(x,t) = Acos(\omega t - kx + \phi) \tag{A1-2}$$

By substituting A1-2 back to equation -A1-1, we can obtain:

$$-k^2 Acos(\omega t - kx + \phi) + \frac{1}{v^2}\omega^2 Acos(\omega t - kx + \phi) = 0 \tag{A1-3}$$

$$\Rightarrow$$

$$v^2 = (\frac{k}{\omega})^2 \tag{A1-4}$$

The right side of A1-4 is just the real definition of wave velocity, and here we can see the reason for why 'v' in equation -A1-1 represents wave velocity.
We return to the topic, the common solution -A1-2 is just what we call *plane wave*. By definition, *plane wave* refers to the wave for which the wavefronts (surface of constant phase) are infinite parallel planes of constant peak-to-peak amplitude normal to the wave velocity vector. Fig. 3. is given to show why A1-2 possesses infinite parallel wavefronts.
From Fig. 3., it can be seen that no matter where the wavefront point is, the projection of wavefront-origin on propagation direction is the same. This means the effective phase delay is the same for every point on the plane which is perpendicular to the propagation direction.
Also by using the complex exponential form, the plane wave function A1-2 can then be expressed as:

$$u(x,t) = e^{i(\omega t - kx + \phi)} \tag{A1-5}$$

which is for the convenience of mathematical expression and calculation.