Quantum Mechanics

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VII. Scattering Theory

7.1 Time-Dependent Perturbation of Scattering

7.1.1 Scattering Matrix

We assume that the Hamiltonian can be written as

$$H = H_0 + V(\mathbf{r}), \tag{7.1}$$

where the kinetic-energy operator

$$H_0 = \frac{\mathbf{p}^2}{2m} \tag{7.2}$$

has the eigenvalues

$$E_k = \frac{\hbar^2 \mathbf{k}^2}{2m} \tag{7.3}$$

and plane-wave eigenvectors $|\mathbf{k}\rangle$, and the scattering potential $V(\mathbf{r})$ is independent of time.

The scattering problem can be analyzed in terms of time-dependent perturbation theory in the interaction picture, which is reviewed below. The initial state $|\alpha, t_0; t_0\rangle_{\mathrm{I}}$ evolves with time as

$$|\alpha, t; t_0\rangle_{\mathrm{I}} = U_{\mathrm{I}}(t, t_0)|\alpha, t_0; t_0\rangle_{\mathrm{I}}, \tag{7.4}$$

where $U_{\mathrm{I}}(t, t_0)$ satisfies the equation

$$i\hbar \frac{\partial}{\partial t} U_{\mathrm{I}}(t, t_0) = V_{\mathrm{I}}(t) U_{\mathrm{I}}(t, t_0) \tag{7.5}$$

with $U_{\mathrm{I}}(t_0, t_0) = 1$ and $V_{\mathrm{I}}(t) = \exp(iH_0 t/\hbar) V \exp(-iH_0 t/\hbar)$. The solution can be formally written as

$$U_{\mathrm{I}}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} V_{\mathrm{I}}(t') U_{\mathrm{I}}(t', t_0) \mathrm{d}t'. \tag{7.6}$$

Therefore, the "transition amplitude" for an initial state $|i\rangle$ to transform into a final state $|n\rangle$, both of which are eigenstates of H_0, is given by

$$\langle n|U_{\mathrm{I}}(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\sum_m \langle n|V|m\rangle \int_{t_0}^{t} \exp(i\omega_{nm}t')\langle m|U_{\mathrm{I}}(t',t_0)|i\rangle \mathrm{d}t', \tag{7.7}$$

where $\langle n|i\rangle = \delta_{ni}$ and $\hbar\omega_{nm} = E_n - E_m$.

To apply the above formalism to scattering theory, the following adjustments are needed:
(1) The "big box" normalization is applied to the initial and final states:

$$\langle \mathbf{x}|\mathbf{k}\rangle = \frac{1}{L^{3/2}}\exp(i\mathbf{k}\cdot\mathbf{x}), \tag{7.8}$$

where L is the side length of the cubic box.
(2) The initial and final states exist only asymptotically. The first-order treatment of Eq. (7.7) requires $\langle m|U_{\mathrm{I}}(t',t_0)|i\rangle = \delta_{mi}$, so

$$\langle n|U_{\mathrm{I}}(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\langle n|V|i\rangle \int_{t_0}^{t} \exp(i\omega_{ni}t')\mathrm{d}t'. \tag{7.9}$$

In this case, as $t\to\infty$, a "transition rate" emerges as Fermi's golden rule. To also accommodate $t_0\to-\infty$, we define a matrix T as follows:

$$\langle n|U_{\mathrm{I}}(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar}T_{ni}\int_{t_0}^{t} \exp(i\omega_{ni}t'+\varepsilon t')\mathrm{d}t', \tag{7.10}$$

where $\varepsilon > 0$ and $t \ll 1/\varepsilon$. These conditions ensure that $\exp(\varepsilon t')$ is close to unity as $t\to\infty$

and that the integrand goes to zero as $t_0\to-\infty$. We need to take $\varepsilon\to 0$ first before $t\to\infty$.

We can now define the **scattering (or S) matrix** in terms of the T matrix:

$$\begin{aligned} S_{ni} &\equiv \lim_{t\to\infty}\left[\lim_{\varepsilon\to 0}\langle n|U_I(t,-\infty)|i\rangle\right] = \delta_{ni} - \frac{i}{\hbar}T_{ni}\int_{-\infty}^{\infty}\exp(i\omega_{ni}t')\mathrm{d}t' \\ &= \delta_{ni} - 2\pi i\delta(E_n - E_i)T_{ni} \end{aligned}. \tag{7.11}$$

It consists of two parts: (1) the final state is the same as the initial state; (2) some soft of scattering governed by the T matrix occurs.

7.1.2 Transition Rates and Cross Sections

The **transition rate** is defined as

$$w(i\to n) = \frac{\mathrm{d}}{\mathrm{d}t}\left|\langle n|U_{\mathrm{I}}(t,-\infty)|i\rangle\right|^2, \tag{7.12}$$

where, for $|i\rangle \neq |n\rangle$, we have

$$\langle n|U_{\mathrm{I}}(t,-\infty)|i\rangle = -\frac{i}{\hbar}T_{ni}\int_{-\infty}^{t}\exp(i\omega_{ni}t'+\varepsilon t')\mathrm{d}t' = -\frac{i}{\hbar}T_{ni}\frac{\exp(i\omega_{ni}t+\varepsilon t)}{i\omega_{ni}+\varepsilon}. \tag{7.13}$$

Therefore

$$w(i\to n) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{\hbar^2}|T_{ni}|^2\frac{\exp(2\varepsilon t)}{\omega_{ni}^2+\varepsilon^2}\right) = \frac{1}{\hbar^2}|T_{ni}|^2\frac{2\varepsilon\exp(2\varepsilon t)}{\omega_{ni}^2+\varepsilon^2}. \tag{7.14}$$

Because

$$\int_{-\infty}^{\infty} \frac{1}{\omega^2 + \varepsilon^2} \mathrm{d}\omega = \frac{\pi}{\varepsilon}, \tag{7.15}$$

for $\varepsilon > 0$ and finite *t*, we have

$$\lim_{\varepsilon \to 0} \frac{\varepsilon \exp(2\varepsilon t)}{\omega_{ni}^2 + \varepsilon^2} = \pi \delta(\omega_{ni}) = \pi \hbar \delta(E_n - E_i). \tag{7.16}$$

So the transition rate is

$$w(i \to n) = \frac{2\pi}{\hbar} |T_{ni}|^2 \delta(E_n - E_i), \tag{7.17}$$

which is independent of time.

With the "big box" normalization, we write

$$E_{\mathbf{n}} = \frac{\hbar^2 \mathbf{k}'^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 |\mathbf{n}|^2, \tag{7.18}$$

so

$$\Delta E_{\mathbf{n}} = \frac{\hbar^2}{m} \left(\frac{2\pi}{L}\right)^2 |\mathbf{n}| \Delta |\mathbf{n}|, \tag{7.19}$$

where $\mathbf{n} = n_x \mathbf{i} + n_y \mathbf{j} + n_z \mathbf{k}$ and $n_{x,y,z}$ are integers. The number of states within a spherical shell of radius $|\mathbf{n}|$ and thickness $\Delta |\mathbf{n}|$ is

$$\Delta n = 4\pi |\mathbf{n}|^2 \Delta |\mathbf{n}| \frac{\mathrm{d}\Omega}{4\pi}, \tag{7.20}$$

so the density of final states

$$\rho(E_n) \equiv \frac{\Delta n}{\Delta E_n} = \frac{m}{\hbar^2} \left(\frac{L}{2\pi}\right)^2 |\mathbf{n}| \mathrm{d}\Omega = \frac{mk}{\hbar^2} \left(\frac{L}{2\pi}\right)^3 \mathrm{d}\Omega. \tag{7.21}$$

Putting into Eq. (7.17), the transition state is given by

$$w(i \to n) = \frac{mkL^3}{(2\pi)^2 \hbar^3} |T_{ni}|^2 \mathrm{d}\Omega. \tag{7.22}$$

A beam of particles with momentum $\hbar \mathbf{k}$ are scattered into a solid angle $\mathrm{d}\Omega$, so the time to cross the "big box" is

$$L / v = mL / \hbar k. \tag{7.23}$$

Thus the probability flux in the particle beam is

$$\mathbf{j}(\mathbf{x}, t) = \frac{1/L^2}{L/v} = v / L^3. \tag{7.24}$$

The **cross section**, defined as the transition rate Eq. (7.22) divided by the flux Eq. (7.24), is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{mL^3}{2\pi\hbar^2}\right)^2 |T_{ni}|^2. \tag{7.25}$$

7.1.3 Solution of the *T* Matrix

From Eq. (7.10) and Eq. (7.13), we have

$$\langle n|U_{\mathrm{I}}(t,-\infty)|i\rangle=\delta_{ni}+\frac{1}{\hbar}T_{ni}\frac{\exp(i\omega_{ni}t+\varepsilon t)}{-\omega_{ni}+i\varepsilon}. \tag{7.26}$$

Insert into Eq. (7.7) with $t_0=-\infty$, and using $\omega_{nm}+\omega_{mi}=\omega_{ni}$, we obtain

$$T_{ni}=V_{ni}+\frac{1}{\hbar}\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}=V_{ni}+\sum_m V_{nm}\frac{T_{mi}}{E_i-E_m+i\hbar\varepsilon}, \tag{7.27}$$

where $V_{nm}=\langle n|V|m\rangle$. Define a set of vectors $\left|\psi^{(+)}\right\rangle$, so that

$$T_{ni}=\left\langle n|V\middle|\psi^{(+)}\right\rangle. \tag{7.28}$$

Eq. (7.27) then becomes

$$\left\langle n|V\middle|\psi^{(+)}\right\rangle=\langle n|V|i\rangle+\sum_m\langle n|V|m\rangle\frac{\left\langle m|V\middle|\psi^{(+)}\right\rangle}{E_i-E_m+i\hbar\varepsilon}, \tag{7.29}$$

which leads to the **Lippmann-Schwinger equation**:

$$\left|\psi^{(+)}\right\rangle=|i\rangle+\sum_m|m\rangle\frac{\left\langle m|V\middle|\psi^{(+)}\right\rangle}{E_i-E_m+i\hbar\varepsilon}=|i\rangle+\frac{V\left|\psi^{(+)}\right\rangle}{E_i-H_0+i\hbar\varepsilon}. \tag{7.30}$$

Eq. (7.25) can be rewritten as

$$\frac{d\sigma}{d\Omega}=\left(\frac{mL^3}{2\pi\hbar^2}\right)^2\left|\left\langle n|V\middle|\psi^{(+)}\right\rangle\right|^2. \tag{7.31}$$

Because $T_{ni}=\langle n|T|i\rangle$, due to Eq. (7.28), we have

$$T|i\rangle=V\left|\psi^{(+)}\right\rangle. \tag{7.32}$$

Operating from the left of Eq. (7.30) with *V*, and using the above equation, we obtain

$$T=V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}T. \tag{7.33}$$

Given the scattering potential *V* is “weak”, the above operator equation can be approximated as

$$T=V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}V\frac{1}{E_i-H_0+i\hbar\varepsilon}V+\cdots. \tag{7.34}$$

If the scattering process evolves backward in time from a plane-wave state $|i\rangle$ in the far future to a state $|n\rangle$ in the distant past, Eq. (7.6) can be rewritten as

$$U_{\mathrm{I}}(t,t_0)=1+\frac{i}{\hbar}\int_t^{t_0}V_{\mathrm{I}}(t')U_{\mathrm{I}}(t',t_0)\mathrm{d}t', \tag{7.35}$$

and Eq. (7.10) becomes

$$\langle n|U_{\mathrm{I}}(t,t_0)|i\rangle=\delta_{ni}+\frac{i}{\hbar}T_{ni}\int_t^{t_0}\exp(i\omega_{ni}t'-\varepsilon t')\mathrm{d}t'. \tag{7.36}$$

In this case, the *T* operator is defined through a set of $\left|\psi^{(-)}\right\rangle$ through $T|i\rangle=V\left|\psi^{(-)}\right\rangle$.

7.2 Scattering Amplitude, Phase Shifts, and Partial Waves

7.2.1 Scattering Amplitude

By replacing $\hbar\varepsilon$ with ε, and denoting the initial (and final) energy in elastic scattering by E, we rewrite Eq. (7.30) as

$$\left|\psi^{(\pm)}\right\rangle = |i\rangle + \frac{V\left|\psi^{(\pm)}\right\rangle}{E - H_0 \pm i\varepsilon}. \tag{7.37}$$

Multiplying $\langle \mathbf{x}|$ from the left and inserting its completeness relation, the above equation leads to

$$\left\langle \mathbf{x}\middle|\psi^{(\pm)}\right\rangle = \langle \mathbf{x}|i\rangle + \int \mathrm{d}^3x' \langle \mathbf{x}|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{x}'\rangle\langle \mathbf{x}'|V\left|\psi^{(\pm)}\right\rangle. \tag{7.38}$$

First evaluate

$$\begin{aligned} G_\pm(\mathbf{x},\mathbf{x}') &= \frac{\hbar^2}{2m}\langle \mathbf{x}|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{x}'\rangle \\ &= \frac{\hbar^2}{2m}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\langle \mathbf{x}|\mathbf{k}'\rangle\langle \mathbf{k}'|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{k}''\rangle\langle \mathbf{k}''|\mathbf{x}'\rangle \end{aligned}. \tag{7.39}$$

Because

$$\langle \mathbf{k}'|\frac{1}{E - H_0 \pm i\varepsilon}|\mathbf{k}''\rangle = \langle \mathbf{k}'|\frac{1}{E - \left(\hbar^2\mathbf{k}'^2/2m\right) \pm i\varepsilon}|\mathbf{k}''\rangle = \frac{\delta_{\mathbf{k}'\mathbf{k}''}}{E - \left(\hbar^2\mathbf{k}'^2/2m\right) \pm i\varepsilon}, \tag{7.40}$$

and using

$$\langle \mathbf{x}|\mathbf{k}'\rangle = \frac{\exp\left(i\mathbf{k}'\cdot\mathbf{x}\right)}{L^{3/2}}, \quad \langle \mathbf{k}''|\mathbf{x}'\rangle = \frac{\exp\left(-i\mathbf{k}''\cdot\mathbf{x}'\right)}{L^{3/2}}, \tag{7.41}$$

Eq. (7.39) becomes

$$G_\pm(\mathbf{x},\mathbf{x}') = \frac{1}{L^3}\sum_{\mathbf{k}'}\frac{\exp\left[i\mathbf{k}'\cdot\left(\mathbf{x}-\mathbf{x}'\right)\right]}{k^2 - k'^2 \pm i\varepsilon}. \tag{7.42}$$

This sum can be converted to integral by taking $L \to \infty$. Since

$$k_i = 2\pi n_i / L, \quad i = x, y, z, \tag{7.43}$$

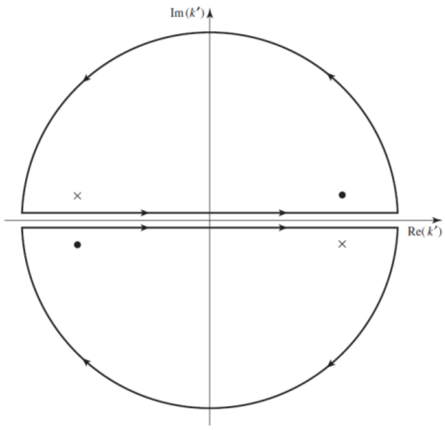
the integral measure becomes $\mathrm{d}^3k' = \left(\frac{2\pi}{L}\right)^3$, so we have

$$G_\pm(\mathbf{x},\mathbf{x}') = \frac{1}{(2\pi)^3}\int \mathrm{d}^3k' \frac{\exp\left[i\mathbf{k}'\cdot\left(\mathbf{x}-\mathbf{x}'\right)\right]}{k^2 - k'^2 \pm i\varepsilon}. \tag{7.44}$$

Converting to spherical coordinates, the integral over $\phi_{k'}$ gives a factor of 2π. Let $\mu \equiv \cos\theta_{k'}$, the above integral becomes

$$
\begin{aligned}
G_{\pm}(\mathbf{x},\mathbf{x}') &= \frac{1}{(2\pi)^2}\int_0^{\infty} k'^2 \mathrm{d}k' \int_{-1}^{+1} \mathrm{d}\mu \frac{\exp\left(ik'|\mathbf{x}-\mathbf{x}'|\mu\right)}{k^2 - k'^2 \pm i\varepsilon} \\
&= \frac{1}{8\pi^2}\frac{1}{i|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty} k'\mathrm{d}k' \left[\frac{\exp\left(ik'|\mathbf{x}-\mathbf{x}'|\right) - \exp\left(-ik'|\mathbf{x}-\mathbf{x}'|\right)}{k^2 - k'^2 \pm i\varepsilon}\right], \\
&= \frac{1}{8\pi^2}\frac{1}{i|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty} k'\mathrm{d}k' \left[\frac{\exp\left(ik'|\mathbf{x}-\mathbf{x}'|\right) - \exp\left(-ik'|\mathbf{x}-\mathbf{x}'|\right)}{-(k'-k_0)(k'+k_0)}\right]
\end{aligned}
\tag{7.45}
$$

where $k_0 \equiv k \pm i\varepsilon$. Treating k' as a complex variable, and taking an integration contour running along the $\mathrm{Re}(k')$ axis, and then closed with a semi-circle in either the upper or lower plane.



Integrating the two terms in (6.44) using complex contours. The dots (crosses) mark the positions of the two poles for the + (−) form of $G_{\pm}(\mathbf{x},\mathbf{x}')$. We replace the integral over a real-valued k' in (6.44) with one of the two contours in the figure, choosing the one on which the factor $e^{\pm ik'|\mathbf{x}-\mathbf{x}'|}$ tends to zero along the semicircle at large $\mathrm{Im}(k')$. Thus, the only contribution to the contour integral is along the real axis.

Using the Cauchy integral formula

$$
\oint_C \frac{f(z)}{z - z_0}\mathrm{d}z = 2\pi i f(z_0), \tag{7.46}
$$

where the contour C is followed counter-clockwise, the first integral in the RHS of Eq. (7.45) becomes

$$
2\pi i(\pm k)\frac{\exp\left[i(\pm k)|\mathbf{x}-\mathbf{x}'|\right]}{\mp 2k} = -\pi i \exp\left[\pm ik|\mathbf{x}-\mathbf{x}'|\right]. \tag{7.47}
$$

The second term is the same because it has another overall minus sign coming from the clockwise trace. Therefore, we finally have

$$
G_{\pm}(\mathbf{x},\mathbf{x}') = -\frac{1}{4\pi}\frac{\exp\left(\pm ik|\mathbf{x}-\mathbf{x}'|\right)}{|\mathbf{x}-\mathbf{x}'|}, \tag{7.48}
$$

which is just Green's function for the Helmholtz equation:

$$
\left(\nabla^2 + k^2\right)G_{\pm}(\mathbf{x},\mathbf{x}') = \delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{7.49}
$$

and the solution of the eigenvalue equation

$$
H_0 G_{\pm} = E G_{\pm} \tag{7.50}
$$

for $\mathbf{x} \neq \mathbf{x}'$.

By using Eq. (7.48), Eq. (7.38) can then be rewrite as

$$\left\langle \mathbf{x} \middle| \psi^{(\pm)} \right\rangle = \langle \mathbf{x} | i \rangle - \frac{2m}{\hbar^2} \int \mathrm{d}^3 x' \frac{\exp\left(\pm ik \left|\mathbf{x}-\mathbf{x}'\right|\right)}{4\pi \left|\mathbf{x}-\mathbf{x}'\right|} \left\langle \mathbf{x}' \middle| V \middle| \psi^{(\pm)} \right\rangle . \tag{7.51}$$

This expression means that the positive (negative) solution corresponds to the plane wave plus an outgoing (incoming) spherical wave.

For the specific case that potential V is local:

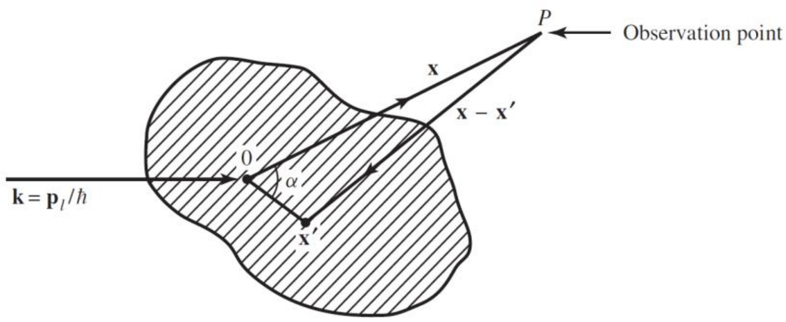
$$\langle \mathbf{x}' | V | \mathbf{x}'' \rangle = V(\mathbf{x}') \delta^{(3)}(\mathbf{x}' - \mathbf{x}''), \tag{7.52}$$

we have

$$\left\langle \mathbf{x}' \middle| V \middle| \psi^{(\pm)} \right\rangle = \int \mathrm{d}^3 x'' \langle \mathbf{x}' | V | \mathbf{x}'' \rangle \left\langle \mathbf{x}'' \middle| \psi^{(\pm)} \right\rangle = V(\mathbf{x}') \left\langle \mathbf{x}' \middle| \psi^{(\pm)} \right\rangle . \tag{7.53}$$

Eq. (7.51) can be simplified as

$$\left\langle \mathbf{x} \middle| \psi^{(\pm)} \right\rangle = \langle \mathbf{x} | i \rangle - \frac{2m}{\hbar^2} \int \mathrm{d}^3 x' \frac{\exp\left(\pm ik \left|\mathbf{x}-\mathbf{x}'\right|\right)}{4\pi \left|\mathbf{x}-\mathbf{x}'\right|} V(\mathbf{x}') \left\langle \mathbf{x}' \middle| \psi^{(\pm)} \right\rangle . \tag{7.54}$$



Finite-range scattering potential. The *observation point P* is where the wave function $\langle \mathbf{x} | \psi^{(\pm)} \rangle$ is to be evaluated, while the contribution to the integral in (6.52) is for $|\mathbf{x}'|$ less than the range of the potential, as depicted by the shaded region of the figure.

Introducing $r = |\mathbf{x}|$, $r' = |\mathbf{x}'|$, and $\alpha = \angle(\mathbf{x}, \mathbf{x}')$, for $r \gg r'$, we have

$$\left|\mathbf{x}-\mathbf{x}'\right| = \sqrt{r^2 - 2rr'\cos\alpha + r'^2} = r\sqrt{1 - \frac{2r'}{r}\cos\alpha + \frac{r'^2}{r^2}} \approx r - \hat{\mathbf{r}} \cdot \mathbf{x}' , \tag{7.55}$$

where $\hat{\mathbf{r}} \equiv \mathbf{x} / |\mathbf{x}|$, which leads to

$$\exp\left(\pm ik\left|\mathbf{x}-\mathbf{x}'\right|\right) \approx \exp(\pm ikr) \exp(\pm i\mathbf{k}' \cdot \mathbf{x}'), \tag{7.56}$$

For large r, where $\mathbf{k}' \equiv k\hat{\mathbf{r}}$.

In summary, for the initial state $|i\rangle = |\mathbf{k}\rangle$, we have

$$\begin{aligned} \left\langle \mathbf{x} \middle| \psi^{(+)} \right\rangle &\xrightarrow{\text{large } r} \langle \mathbf{x} | \mathbf{k} \rangle - \frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{\exp(ikr)}{r} \int \mathrm{d}^3 x' \exp(-i\mathbf{k}' \cdot \mathbf{x}') V(\mathbf{x}') \left\langle \mathbf{x}' \middle| \psi^{(+)} \right\rangle \\ &= \frac{1}{L^{3/2}} \left[\exp(i\mathbf{k} \cdot \mathbf{x}) + \frac{\exp(ikr)}{r} f(\mathbf{k}', \mathbf{k}) \right] \end{aligned} , \tag{7.57}$$

which illustrates the original plane wave in propagation direction **k** plus an outgoing spherical wave with the **scattering amplitude**

$$f\left(\mathbf{k}',\mathbf{k}\right) \equiv -\frac{1}{4\pi}\frac{2m}{\hbar^2}L^3\int \mathrm{d}^3x' \frac{\exp\left(-i\mathbf{k}'\cdot\mathbf{x}'\right)}{L^{3/2}}V\left(\mathbf{x}'\right)\left\langle \mathbf{x}'\middle|\psi^{(+)}\right\rangle = -\frac{mL^3}{2\pi\hbar^2}\left\langle \mathbf{k}'\middle|V\middle|\psi^{(+)}\right\rangle . \quad (7.58)$$

By comparing with Eq. (7.31), the differential cross section can be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left|f\left(\mathbf{k}',\mathbf{k}\right)\right|^2 . \quad (7.59)$$

The more realistic situation should consider a wave packet, but a plane wave is satisfactory if the dimension of the wave packet is much larger than the size of the scatterer.

The optical theorem:

$$\operatorname{Im} f\left(\theta = 0\right) = \frac{k}{4\pi}\sigma_{\text{tot}} , \quad (7.60)$$

where $f\left(\theta=0\right) \equiv f\left(\mathbf{k},\mathbf{k}\right)$ and $\sigma_{\text{tot}} \equiv \int \mathrm{d}\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$.

Proof: Start with the Lippman-Schwinger Equation Eq. (7.37) with $\left|i\right\rangle = \left|\mathbf{k}\right\rangle$ to write

$$\left\langle \mathbf{k}\right| = \left\langle \psi^{(+)}\right| - \frac{\left\langle \psi^{(+)}\right|V}{E - H_0 - i\varepsilon} , \quad (7.61)$$

so

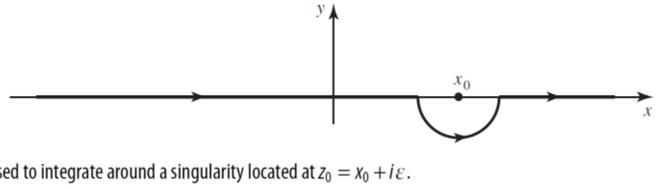
$$\begin{aligned} \left\langle \mathbf{k}\middle|V\middle|\psi^{(+)}\right\rangle &= \left(\left\langle \psi^{(+)}\right| - \left\langle \psi^{(+)}\right|V\frac{1}{E - H_0 - i\varepsilon}\right)V\left|\psi^{(+)}\right\rangle \\ &= \left\langle \psi^{(+)}\middle|V\middle|\psi^{(+)}\right\rangle - \left\langle \psi^{(+)}\middle|V\frac{1}{E - H_0 - i\varepsilon}V\middle|\psi^{(+)}\right\rangle \end{aligned} . \quad (7.62)$$

The first term at the RHS is real since it is the expectation value of a Hermitian operator. To solve the second term, we use the concept of the Cauchy principal value in complex integration:

$$\begin{aligned} \int_{-\infty}^{\infty}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x &= \int_{-\infty}^{x_0-\delta}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x + \int_c \frac{f\left(z\right)}{z - z_0}\mathrm{d}z + \int_{x_0+\delta}^{\infty}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x = 0 \\ &= \mathscr{P}\int_{-\infty}^{\infty}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x + \int_c \frac{f\left(z\right)}{z - z_0}\mathrm{d}z \end{aligned} , \quad (7.63)$$

where the Cauchy principle value is defined as

$$\mathscr{P}\int_{-\infty}^{\infty}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x = \lim_{\delta\to 0}\left\{\int_{-\infty}^{x_0-\delta}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x + \int_{x_0+\delta}^{\infty}\frac{f\left(x\right)}{x - x_0}\mathrm{d}x\right\} . \quad (7.64)$$



Contour used to integrate around a singularity located at $z_0 = x_0 + i\varepsilon$.

Since

$$\int_c \frac{f(z)}{z-z_0}\mathrm{d}z = i\pi f(x_0), \tag{7.65),}$$

Eq. (7.63) becomes

$$\int_{-\infty}^{\infty}\frac{f(x)}{x-x_0}\mathrm{d}x = \mathscr{P}\int_{-\infty}^{\infty}\frac{f(x)}{x-x_0}\mathrm{d}x + i\pi f(x_0). \tag{7.66}$$

Using the above equation, the term in Eq. (7.62)

$$\lim_{\varepsilon\to 0}\left(\frac{1}{E-H_0-i\varepsilon}\right) = \lim_{\varepsilon\to 0}\int_{-\infty}^{\infty}\frac{\delta(E-E')}{E'-H_0-i\varepsilon}\mathrm{d}E' = i\pi\delta(E-H_0). \tag{7.67}$$

Therefore, we obtain

$$\mathrm{Im}\langle\mathbf{k}|V|\psi^{(+)}\rangle = -\pi\langle\psi^{(+)}|V\delta(E-H_0)V|\psi^{(+)}\rangle = -\pi\langle\mathbf{k}|T^\dagger\delta(E-H_0)T|\mathbf{k}\rangle. \tag{7.68}$$

Using Eq. (7.58), we have

$$\begin{aligned}\mathrm{Im}\, f(\mathbf{k},\mathbf{k}) &= -\frac{mL^3}{2\pi\hbar^2}\mathrm{Im}\langle\mathbf{k}|V|\psi^{(+)}\rangle = \frac{mL^3}{2\hbar^2}\langle\mathbf{k}|T^\dagger\delta(E-H_0)T|\mathbf{k}\rangle \\ &= \frac{mL^3}{2\hbar^2}\sum_{\mathbf{k}'}\langle\mathbf{k}|T^\dagger\delta(E-H_0)|\mathbf{k}'\rangle\langle\mathbf{k}'|T|\mathbf{k}\rangle \\ &= \frac{mL^3}{2\hbar^2}\sum_{\mathbf{k}'}\left|\langle\mathbf{k}'|T|\mathbf{k}\rangle\right|^2\delta_{k,k'}\end{aligned}. \tag{7.69}$$

Finally, applying $\langle\mathbf{k}'|\mathbf{T}|\mathbf{k}\rangle = \langle\mathbf{k}'|\mathbf{V}|\psi^{(+)}\rangle$ to Eq. (7.58), the above equation becomes

$$\begin{aligned}\mathrm{Im}\, f(\mathbf{k},\mathbf{k}) &= \frac{mL^3}{2\hbar^2}\left(\frac{2\pi\hbar^2}{mL^3}\right)^2\sum_{\mathbf{k}'}\left|f(\mathbf{k}',\mathbf{k})\right|^2\delta_{k,k'} \\ &\to \frac{2\pi^2\hbar^2}{m(2\pi)^3}\int \mathrm{d}^3k'\left|f(\mathbf{k}',\mathbf{k})\right|^2\delta\left(E-\frac{\hbar^2\mathbf{k}'^2}{2m}\right) \\ &= \frac{\hbar^2}{4\pi m}\frac{m}{\hbar^2 k}k^2\int \mathrm{d}\Omega_{k'}\frac{d\sigma}{\mathrm{d}\Omega_{k'}} \\ &= \frac{k}{4\pi}\sigma_{\mathrm{tot}}\end{aligned}. \tag{7.70}$$

7.2.2 Free-Particle States

A **spherical-wave state**, denoted by $|E,l,m\rangle$, is the simultaneous eigenstate of H_0, $\mathbf{L}^2$, and L_z. A free-particle state can be analyzed using either the plane-wave basis $\{|k\rangle\}$ or the spherical-wave basis $\{|E,l,m\rangle\}$.

The transformation function can be written as

$$\langle\mathbf{k}|E,l,m\rangle = g_{lE}(k)Y_l^m(\hat{\mathbf{k}}). \tag{7.71}$$

To determine $g_{lE}(k)$, we first note that

$$\left(H_0-E\right)\left|E,l,m\right\rangle=0 \tag{7.72}$$

and

$$\left\langle\mathbf{k}\right|\left(H_0-E\right)=\left(\frac{\hbar^2k^2}{2m}-E\right)\left\langle\mathbf{k}\right|. \tag{7.73}$$

Multiplied by $\left|E,l,m\right\rangle$ on the right, we obtain

$$\left(\frac{\hbar^2k^2}{2m}-E\right)\left\langle\mathbf{k}\middle|E,l,m\right\rangle=0\,. \tag{7.74}$$

Therefore, $g_{lE}\left(k\right)$ can be written as

$$g_{lE}\left(k\right)=N\delta\left(\frac{\hbar^2k^2}{2m}-E\right), \tag{7.75}$$

where N may be determined by the normalization convention

$$\left\langle E',l',m'\middle|E,l,m\right\rangle=\delta_{ll'}\delta_{mm'}\delta\left(E-E'\right) \tag{7.76}$$

through

$$\begin{aligned}
&\left\langle E',l',m'\middle|E,l,m\right\rangle=\int\mathrm{d}^3k''\left\langle E',l',m'\middle|\mathbf{k}''\right\rangle\left\langle\mathbf{k}''\middle|E,l,m\right\rangle\\
&=\int k''^2\mathrm{d}k''\int\mathrm{d}\Omega_{\mathbf{k}''}\left|N\right|^2\delta\left(\frac{\hbar^2k''^2}{2m}-E'\right)\delta\left(\frac{\hbar^2k''^2}{2m}-E\right)Y_{l'}^{m'*}\left(\hat{\mathbf{k}}''\right)Y_l^m\left(\hat{\mathbf{k}}''\right)\\
&=\int\frac{k''^2\mathrm{d}E''}{\mathrm{d}E''/\mathrm{d}k''}\int d\Omega_{\mathbf{k}''}\left|N\right|^2\delta\left(\frac{\hbar^2k''^2}{2m}-E'\right)\delta\left(\frac{\hbar^2k''^2}{2m}-E\right)Y_{l'}^{m'*}\left(\hat{\mathbf{k}}''\right)Y_l^m\left(\hat{\mathbf{k}}''\right),\\
&=\left|N\right|^2\frac{mk'}{\hbar^2}\delta\left(E-E'\right)\delta_{ll'}\delta_{mm'}
\end{aligned} \tag{7.77}$$

which gives

$$N=\hbar/\sqrt{mk}\,. \tag{7.78}$$

Hence

$$g_{lE}\left(k\right)=\frac{\hbar}{\sqrt{mk}}\delta\left(\frac{\hbar^2k^2}{2m}-E\right), \tag{7.79}$$

and thus the wave function for $\left|E,l,m\right\rangle$ in momentum space is

$$\left\langle\mathbf{k}\middle|E,l,m\right\rangle=\frac{\hbar}{\sqrt{mk}}\delta\left(\frac{\hbar^2k^2}{2m}-E\right)Y_l^m\left(\hat{\mathbf{k}}\right). \tag{7.80}$$

The plane-wave state can then be written as

$$\left|\mathbf{k}\right\rangle=\sum_l\sum_m\int\mathrm{d}E\left|E,l,m\right\rangle\left\langle E,l,m\middle|\mathbf{k}\right\rangle=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left|E,l,m\right\rangle\Big|_{E=\hbar^2k^2/2m}\left(\frac{\hbar}{\sqrt{mk}}Y_l^{m*}\left(\hat{\mathbf{k}}\right)\right). \tag{7.81}$$

Next, we consider the corresponding wave function in position space. The wave function for a spherical wave is $j_l(kr)Y_l^m(\hat{\mathbf{r}})$, where $j_l(kr)$ is the spherical Bessel function of order *l*. Thus we can write

$$\langle \mathbf{x} | E,l,m \rangle = c_l j_l(kr) Y_l^m(\hat{\mathbf{r}}) . \tag{7.82}$$

On the one hand, we have

$$\begin{aligned}
\langle \mathbf{x} | \mathbf{k} \rangle = \frac{\exp(i\mathbf{k}\cdot\mathbf{x})}{(2\pi)^{3/2}} &= \sum_l \sum_m \int \mathrm{d}E \langle \mathbf{x} | E,l,m \rangle \langle E,l,m | \mathbf{k} \rangle \\
&= \sum_l \sum_m \int \mathrm{d}E c_l j_l(kr) Y_l^m(\hat{\mathbf{r}}) \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m} \right) Y_l^{m*}(\hat{\mathbf{k}}), \\
&= \sum_l \frac{(2l+1)}{4\pi} P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}) \frac{\hbar}{\sqrt{mk}} c_l j_l(kr)
\end{aligned} \tag{7.83}$$

where we have used the addition theorem

$$\sum_m Y_l^m(\hat{\mathbf{r}}) Y_l^{m*}(\hat{\mathbf{k}}) = \left[(2l+1)/4\pi \right] P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}), \tag{7.84}$$

On the other hand, by using the following integral representation

$$j_l(kr) = \frac{1}{2i^l} \int_{-1}^{1} \exp(ikr\cos\theta) P_l(\cos\theta) \mathrm{d}(\cos\theta), \tag{7.85}$$

We have

$$\frac{\exp(i\mathbf{k}\cdot\mathbf{x})}{(2\pi)^{3/2}} = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) i^l j_l(kr) P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}) . \tag{7.86}$$

Comparing Eq. (7.83) with Eq. (7.86), we obtain

$$j_l(kr) = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}} . \tag{7.87}$$

To summarize, we have

$$\langle \mathbf{k} | E,l,m \rangle = \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m} \right) Y_l^m(\hat{\mathbf{k}}) \tag{7.88}$$

and

$$\langle \mathbf{x} | E,l,m \rangle = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}} j_l(kr) Y_l^m(\hat{\mathbf{r}}) . \tag{7.89}$$

7.2.3 Partial-Wave Expansion

In case that the potential V is spherically symmetrical, the transition operator T, given by Eq. (7.34), commutes with $\mathbf{L}^2$ and $\mathbf{L}$. It can be proved that

$$\langle E',l',m' | T | E,l,m \rangle = T_l(E) \delta_{ll'} \delta_{mm'} . \tag{7.90}$$

The scattering amplitude Eq. (7.58) becomes

$$
\begin{aligned}
f(\mathbf{k}',\mathbf{k}) &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}L^3\langle\mathbf{k}'|T|\mathbf{k}\rangle \\
&= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\sum_l\sum_m\sum_{l'}\sum_{m'}\int \mathrm{d}E\int \mathrm{d}E'\langle\mathbf{k}'|E'l'm'\rangle\langle E'l'm'|T|Elm\rangle\langle Elm|\mathbf{k}\rangle \\
&= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\frac{\hbar^2}{mk}\sum_l\sum_m T_l(E)\Big|_{E=\hbar^2k^2/2m} Y_l^m(\hat{\mathbf{k}}')Y_l^{m*}(\hat{\mathbf{k}}) \\
&= -\frac{4\pi^2}{k}\sum_l\sum_m T_l(E)\Big|_{E=\hbar^2k^2/2m} Y_l^m(\hat{\mathbf{k}}')Y_l^{m*}(\hat{\mathbf{k}})
\end{aligned} \quad . \qquad (7.91)
$$

By choosing $\mathbf{k}$ to be in the positive z-direction and using $P_l(1)=1$, we have

$$Y_l^m(\hat{\mathbf{k}}) = \sqrt{\frac{2l+1}{4\pi}}\delta_{m0}\,. \qquad (7.92)$$

Taking θ to be the angle between $\mathbf{k}'$ and $\mathbf{k}$, we can write

$$Y_l^0(\hat{\mathbf{k}}') = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)\,. \qquad (7.93)$$

Define the **partial-wave amplitude**:

$$f_l(k) \equiv -\frac{\pi T_l(E)}{k}\,, \qquad (7.94)$$

Eq. (7.91) becomes

$$f(\mathbf{k}',\mathbf{k}) = f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta)\,. \qquad (7.95)$$

According to Eq. (7.86) and $i^l = \exp\left(\frac{i\pi}{2}l\right)$, we have

$$j_l(kr) \xrightarrow{\text{large } r} \frac{1}{2ikr}\left[\exp\left(i\left(kr-\frac{l\pi}{2}\right)\right) - \exp\left(-i\left(kr-\frac{l\pi}{2}\right)\right)\right], \qquad (7.96)$$

So Eq. (7.57) becomes

$$
\begin{aligned}
\langle\mathbf{x}|\psi^{(+)}\rangle &\xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}}\left[\exp(ikz) + f(\theta)\frac{\exp(ikr)}{r}\right] \\
&= \frac{1}{(2\pi)^{3/2}}[\sum_l(2l+1)P_l(\cos\theta)\frac{1}{2ikr}\left[\exp(ikr) - \exp(-i(kr-l\pi))\right] \\
&+ \sum_l(2l+1)f_l(k)P_l(\cos\theta)\frac{\exp(ikr)}{r}] \\
&= \frac{1}{(2\pi)^{3/2}}\sum_l(2l+1)\frac{P_l}{2ik}\left[\left[1+2ikf_l(k)\right]\frac{\exp(ikr)}{r} - \frac{\exp(-i(kr-l\pi))}{r}\right]
\end{aligned} \quad . \qquad (7.97)
$$

The above equation indicates that, in the absence of the scatterer, the plane wave can be treated as the sum of a spherically outgoing wave behaving like $\frac{\exp(ikr)}{r}$ and a spherically incoming wave behaving like $-\frac{\exp[-i(kr-l\pi)]}{r}$ for each l. The presence of the scatterer only changes the outgoing wave:

$$1 \to 1 + 2ikf_l(k) \qquad (7.98)$$

and the incoming wave is completely unaffected.

7.2.4 Unitarity and Phase Shifts

In a time-independent formulation, the flux current density **j** must satisfy

$$\nabla\cdot\mathbf{j}=-\frac{\partial|\psi|^2}{\partial t}=0\,. \tag{7.99}$$

By Gauss's theorem, for a spherical surface of very large radius *S*, we must have

$$\int_S \mathbf{j}\cdot d\mathbf{S}=0\,. \tag{7.100}$$

Because of angular-momentum conservation, this must hold for each partial wave separately. Define

$$S_l(k)\equiv 1+2ikf_l(k)\,, \tag{7.101}$$

from Eq. (7.98), we have the **unitarity relation** for the *l*th partial wave:

$$|S_l(k)|=1\,. \tag{7.102}$$

Therefore, the only change in the wave function at a large distance is in the phase of the outgoing wave. We can write

$$S_l=\exp(2i\delta_l)\,, \tag{7.103}$$

where δ_l is real. According to Eq. (7.101), we have

$$f_l=\frac{S_l-1}{2ik}=\frac{\exp(2i\delta_l)-1}{2ik}=\frac{\exp(i\delta_l)\sin\delta_l}{k}=\frac{1}{k\cot\delta_l-ik}\,. \tag{7.104}$$

The **full scattering amplitude**

$$\begin{aligned}f(\theta)&=\sum_{l=0}(2l+1)\left(\frac{\exp(2i\delta_l)-1}{2ik}\right)P_l(\cos\theta)\\&=\frac{1}{k}\sum_{l=0}(2l+1)\exp(i\delta_l)\sin\delta_l P_l(\cos\theta)\end{aligned}\,, \tag{7.105}$$

which rests on the twin principles of **rotational invariant** and **probability conservation**.

The total cross section

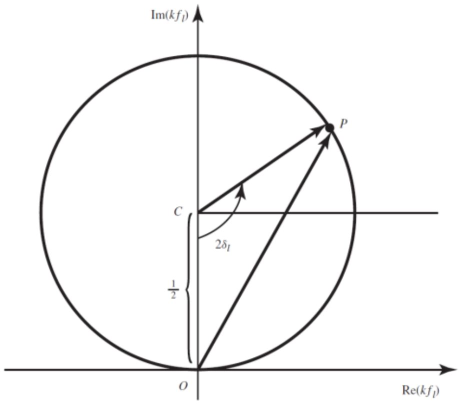
$$\begin{aligned}\sigma_{\text{tot}}&=\int|f(\theta)|^2\,\mathrm{d}\Omega=\frac{1}{k^2}\int_0^{2\pi}\mathrm{d}\phi\int_{-1}^{1}\mathrm{d}(\cos\theta)\sum_l\sum_{l'}(2l+1)(2l'+1)\\&\times\exp(i\delta_l)\sin\delta_l\exp(-i\delta_{l'})\sin\delta_{l'}P_lP_{l'}\\&=\frac{4\pi}{k^2}\sum_l(2l+1)\sin^2\delta_l\end{aligned}\,, \tag{7.106}$$

which satisfies the optical theorem Eq. (7.60).

From Eq. (7.104), we know

$$kf_l=\frac{i}{2}+\frac{1}{2}\exp\left(-\frac{i\pi}{2}+2i\delta_l\right), \tag{7.107}$$

which indicates that kf_l must lie on the unitary circle of radius 1/2.



Argand diagram for kf_l. OP is the magnitude of kf_l, while CO and CP are each radii of length $\frac{1}{2}$ on the unitary circle; angle $OCP = 2\delta_l$.

If δ_l is small, f_l must stay near the bottom of the circle and is almost purely real:

$$f_l = \frac{\exp(i\delta_l)\sin\delta_l}{k} \simeq \frac{(1+i\delta_l)\delta_l}{k} \simeq \frac{\delta_l}{k}. \tag{7.108}$$

On the other hand, if δ_l is near $\pi/2$, kf_l is almost purely imaginary with the magnitude maximal. The maximum partial cross section

$$\sigma_{\max}^{(l)} = 4\pi\lambda\!\!\bar{}^{\,2}(2l+1) \tag{7.109}$$

is achieved when $\sin^2\delta_l = 1$.

7.2.5 Determination of Phase Shifts

Considering a given potential $V(r)$ which vanishes when r is beyond a certain range R, where the wave function must be that of a free spherical wave. Because the origin is excluded from our consideration, we should count in the solution of $n_l(r)$ besides $j_l(r)$. Define the spherical Hankel functions

$$h_l^{(1)} = j_l + in_l, \quad h_l^{(2)} = j_l - in_l, \tag{7.110}$$

which have the asymptotic behavior

$$h_l^{(1)} \xrightarrow{\text{large } r} \frac{\exp[i(kr - l\pi/2)]}{ikr}, \quad h_l^{(2)} \xrightarrow{\text{large } r} -\frac{\exp[-i(kr - l\pi/2)]}{ikr}. \tag{7.111}$$

The full-wave function at $r > R$ can be written as

$$\langle \mathbf{x} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} \sum i^l (2l+1) A_l(r) P_l(\cos\theta), \tag{7.112}$$

Where the radial-wave function

$$A_l(r) = c_l^{(1)} h_l^{(1)}(kr) + c_l^{(2)} h_l^{(2)}(kr). \tag{7.113}$$

Due to Eq. (7.111), Eq. (7.112) should compare with

$$\frac{1}{(2\pi)^{3/2}}\sum_l (2l+1)P_l\left[\frac{\exp(2i\delta_l)\exp(ikr)}{2ikr}-\frac{\exp[-i(kr-l\pi)]}{2ikr}\right], \tag{7.114}$$

so we must have

$$c_l^{(1)}=\frac{1}{2}\exp(2i\delta_l),\quad c_l^{(2)}=\frac{1}{2}. \tag{7.115}$$

The radial-wave function for $r>R$ is thus

$$A_l(r)=\exp(i\delta_l)\left[\cos\delta_l\, j_l(kr)-\sin\delta_l n_l(kr)\right]. \tag{7.116}$$

The logarithmic derivative at $r=R$ is

$$\beta_l\equiv\left(\frac{r}{A_l}\frac{\mathrm{d}A_l}{\mathrm{d}r}\right)_{r=R}=kR\left[\frac{j_l'(kR)\cos\delta_l-n_l'(kR)\sin\delta_l}{j_l(kR)\cos\delta_l-n_l(kR)\sin\delta_l}\right], \tag{7.117}$$

which can determine the phase shift as

$$\tan\delta_l=\frac{kRj_l'(kR)-\beta_l j_l(kR)}{kRn_l'(kR)-\beta_l n_l(kR)}. \tag{7.118}$$

Looking at solving the Schrödinger equation with spherically symmetrical potential for $r<R$, the equivalent one-dimensional equation is

$$\frac{\mathrm{d}^2u_l}{\mathrm{d}r^2}+\left(k^2-\frac{2m}{\hbar^2}V-\frac{l(l+1)}{r^2}\right)u_l=0, \tag{7.119}$$

where

$$u_l=rA_l(r) \tag{7.120}$$

subject to the boundary condition

$$u_l\big|_{r=0}=0. \tag{7.121}$$

At $r=R$, we must have β_l continuous. The β_l at $r<R$ can be obtained by integrating Eq. (7.119), and that at $r>R$ can be expressed in terms of the phase shifts characterizing the large-distance behavior of the wave function. The phase shifts can thus be calculated.

7.2.6 Hard-Sphere Scattering

The scatterer is a hard sphere

$$V=\begin{cases}\infty, & r<R\\ 0 & r>R\end{cases}. \tag{7.122}$$

The wave function must vanish at $r=R$, so

$$A_l(r)\big|_{r=R}=0 \tag{7.123}$$

or, from Eq. (7.116),

$$j_l(kR)\cos\delta_l-n_l(kR)\sin\delta_l=0, \tag{7.124}$$

which gives

$$\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}. \tag{7.125}$$

Therefore, the phase shifts are now known for any *l*.

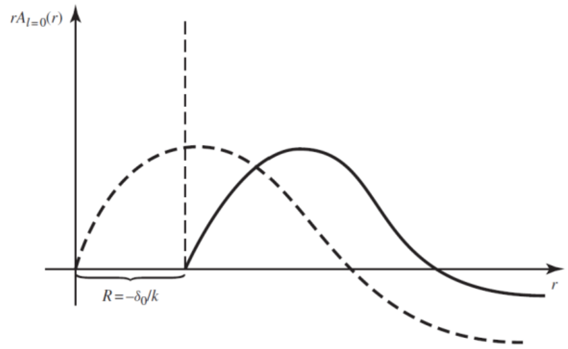
For $l=0$, we have

$$\tan\delta_0 = \frac{\sin kR / kR}{-\cos kR / kR} = -\tan kR \Rightarrow \delta_0 = -kR\ . \tag{7.126}$$

The radial-wave function Eq. (7.116) with $\exp(i\delta_0)$ omitted varies as

$$A_{l=0}(r) \propto \frac{\sin kr}{kr}\cos\delta_0 + \frac{\cos kr}{kr}\sin\delta_0 = \frac{1}{kr}\sin(kr+\delta_0)\,, \tag{7.127}$$

which is shifted from the free sinusoidal wave by amount R.



Plot of $rA_{l=0}(r)$ versus r (with the $e^{i\delta_0}$ factor removed). The dashed curve for $V=0$ behaves like sin kr, while the solid curve is for S-wave hard-sphere scattering, shifted by $R=-\delta_0/k$ from the case $V=0$.

At the low-energy limit $kR \ll 1$,

$$\begin{aligned} j_l(kr) &\simeq \frac{(kr)^l}{(2l+1)!!} \\ n_l(kr) &\simeq -\frac{(2l-1)!!}{(kr)^{l+1}} \end{aligned}, \tag{7.128}$$

so

$$\tan\delta_l = \frac{-(kR)^{2l+1}}{(2l+1)\left[(2l-1)!!\right]^2}\,. \tag{7.129}$$

It is therefore all right to ignore δ_l with $l \neq 0$, namely, we have S-wave scattering only. Using Eq. (7.126), we obtain

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\sin^2\delta_0}{k^2} \simeq R^2\,. \tag{7.130}$$

The total cross section

$$\sigma_{\text{tot}} = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega = 4\pi R^2 \tag{7.131}$$

is four times the geometric cross section πR^2.

7.3 The Born and Eikonal Approximations

7.3.1 The First-Order Born Approximation

Calculating the scattering amplitude $f(\mathbf{k}',\mathbf{k})$ amounts to calculating the matrix element

$$\left\langle \mathbf{k}' \middle| V \middle| \psi^{(+)} \right\rangle = \left\langle \mathbf{k}' \middle| T \middle| \mathbf{k} \right\rangle, \tag{7.132}$$

which can only be analytically solved with some approximations.

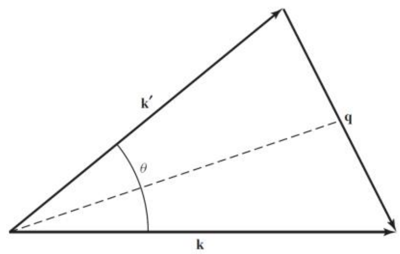
By replacing $\hbar\varepsilon$ with ε, Eq. (7.34) becomes

$$T = V + V\frac{1}{E_i - H_0 + i\varepsilon}V + V\frac{1}{E_i - H_0 + i\varepsilon}V\frac{1}{E_i - H_0 + i\varepsilon}V + \cdots. \tag{7.133}$$

The first term of the above expansion is called the **first-order Born approximation** with $T = V$ and $\left|\psi^{(+)}\right\rangle = |\mathbf{k}\rangle$, where

$$f^{(1)}(\mathbf{k}',\mathbf{k}) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x' \exp\left[i(\mathbf{k}-\mathbf{k}')\cdot x'\right]V(\mathbf{x}') \tag{7.134}$$

is obtained by inserting a complete set of $|\mathbf{x}'\rangle$ into Eq. (7.58), which, apart from an overall factor, is just the 3D Fourier transform of V with respect to $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$.



Scattering through angle θ, where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$.

An important special case is when V is a spherically symmetrical potential. Because $|\mathbf{k}'| = k$ by energy conservation, we have

$$q = |\mathbf{k} - \mathbf{k}'| = 2k\sin\frac{\theta}{2}. \tag{7.135}$$

In this case, Eq. (7.134) can be integrated explicitly as

$$\begin{aligned} f^{(1)}(\theta) &= -\frac{1}{2}\frac{2m}{\hbar^2}\frac{1}{iq}\int_0^\infty \frac{r^2}{r}V(r)\big(\exp(iqr) - \exp(-iqr)\big)\mathrm{d}r \\ &= -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty rV(r)\sin qr\mathrm{d}r \end{aligned}. \tag{7.136}$$

This first Born amplitude with a spherically symmetrical potential has the following properties:

(1) $f^{(1)}(\theta)$ is a function of q only.

(2) $f^{(1)}(\theta)$ is always real.

(3) $\dfrac{d\sigma}{d\Omega}$ is independent of the sign of V.

(4) For small k, and thus small q,

$$f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int V(r)\mathrm{d}^3x \tag{7.137}$$

is independent of θ.

(5) $f^{(1)}(\theta)$ is small for large q because of rapid oscillation of the integrand.

Example 1: Scattering by a finite square well

$$V(r) = \begin{cases} V_0 & r \le a \\ 0 & r > a \end{cases}. \tag{7.138}$$

The integral in Eq. (7.136) then yields

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left(\frac{\sin qa}{qa} - \cos qa\right). \tag{7.139}$$

Example 2: Scattering by a Yukawa potential

$$V(r) = \frac{V_0 \exp(-\mu r)}{\mu r}, \tag{7.140}$$

where V_0 is independent of r and V goes to zero very rapidly for $r \gg 1/\mu$. From Eq. (7.136), by using

$$\sin qr = \mathrm{Im}\left[\exp(iqr)\right] \tag{7.141}$$

and

$$\mathrm{Im}\left[\int_0^\infty \exp(-\mu r)\exp(iqr)\mathrm{d}r\right] = -\mathrm{Im}\left(\frac{1}{-\mu + iq}\right) = \frac{q}{\mu^2 + q^2}, \tag{7.142}$$

we obtain

$$f^{(1)}(\theta) = -\left(\frac{2mV_0}{\mu\hbar^2}\right)\frac{1}{q^2 + \mu^2}. \tag{7.143}$$

Note that

$$q^2 = 4k^2 \sin^2\frac{\theta}{2} = 2k^2(1 - \cos\theta), \tag{7.144}$$

so the differential cross section for scattering by a Yukawa potential in the first Born approximation is given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \simeq \left(\frac{2mV_0}{\mu\hbar^2}\right)^2 \frac{1}{\left[2k^2(1-\cos\theta) + \mu^2\right]^2}. \tag{7.145}$$

As $\mu \to 0$ while keeping V_0/μ fixed to be $ZZ'e^2$, the Yukawa potential is reduced to the Coulomb potential, the differential cross section becomes

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \simeq \frac{(2m)^2(ZZ'e^2)^2}{\hbar^4}\frac{1}{16k^4\sin^4(\theta/2)}. \tag{7.146}$$

Because the kinetic energy $E_{\mathrm{K}} = \frac{|\mathbf{p}|^2}{2m} = \frac{\hbar^2 k^2}{2m}$, the above equation can be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \simeq \frac{1}{16}\left(\frac{ZZ'e^2}{E_{\mathrm{K}}}\right)^2 \frac{1}{\sin^4(\theta/2)}, \tag{7.147}$$

which is exactly the Rutherford scattering cross section obtained *classically*.

7.3.2 Conditions for the Born Approximation to be valid

Eq. (7.51) can be slightly rewritten as

$$\langle \mathbf{x}|\psi^{(+)}\rangle = \langle \mathbf{x}|\mathbf{k}\rangle - \frac{2m}{\hbar^2}\int \mathrm{d}^3x' \frac{\exp(ik|\mathbf{x}-\mathbf{x}'|)}{4\pi|\mathbf{x}-\mathbf{x}'|} V(\mathbf{x}')\langle \mathbf{x}'|\psi^{(+)}\rangle. \tag{7.148}$$

The approximation is that $T \approx V$, which means that $|\psi^{(+)}\rangle$ can be replaced by $|\mathbf{k}\rangle$, so the second term on the RHS must be much smaller than the first one. Assuming that $V(\mathbf{x}) \simeq V_0$ acting with some "range" a and let $r' \equiv |\mathbf{x}-\mathbf{x}'|$, the validity condition is

$$\left|\frac{2m}{\hbar^2}\left(\frac{4\pi}{3}a^3\right)\frac{\exp(ikr')}{4\pi a}V_0 \frac{\exp(i\mathbf{k}\cdot\mathbf{x}')}{L^{3/2}}\right| \ll \left|\frac{\exp(i\mathbf{k}\cdot\mathbf{x})}{L^{3/2}}\right|. \tag{7.149}$$

For low energies $ka \ll 1$, the exponential factors can be replaced by unity, so we obtain the succinct criterion:

$$\frac{m|V_0|a^2}{\hbar^2} \ll 1. \tag{7.150}$$

For high energies $ka \gg 1$, it can be shown that the criterion becomes

$$\frac{2m}{\hbar^2}\frac{|V_0|a}{k}\ln(ka) \ll 1. \tag{7.151}$$

Generally, *the Born approximation tends to get better at higher energies*.

7.3.3 The Higher-Order Born Approximation

To the second order approximation, Eq. (7.133) becomes

$$T = V + V\frac{1}{E - H_0 + i\varepsilon}V. \tag{7.152}$$

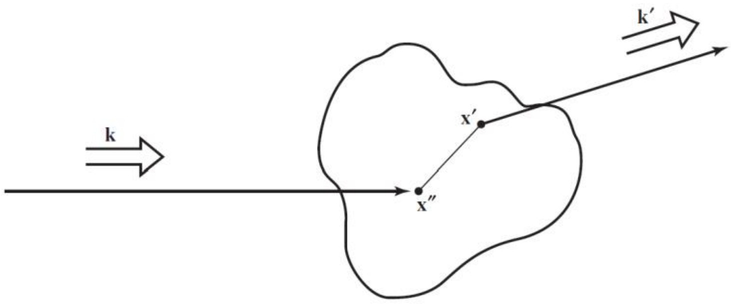
The scattering amplitude

$$f(\mathbf{k}',\mathbf{k}) \approx f^{(1)}(\mathbf{k}',\mathbf{k}) + f^{(2)}(\mathbf{k}',\mathbf{k}) \tag{7.153}$$

with

$$\begin{aligned} f^{(2)}(\mathbf{k}',\mathbf{k}) &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \\ &\times \int \mathrm{d}^3x' \int \mathrm{d}^3x'' \langle \mathbf{k}'|\mathbf{x}'\rangle V(\mathbf{x}')\langle \mathbf{x}'|\frac{1}{E-H_0+i\varepsilon}|\mathbf{x}''\rangle V(\mathbf{x}'')\langle \mathbf{x}''|\mathbf{k}\rangle \\ &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int \mathrm{d}^3x' \int \mathrm{d}^3x'' \exp(-i\mathbf{k}'\cdot\mathbf{x}')V(\mathbf{x}')\left[\frac{2m}{\hbar^2}G_+(\mathbf{x}',\mathbf{x}'')\right]V(\mathbf{x}'')\exp(i\mathbf{k}\cdot\mathbf{x}'') \end{aligned}. \tag{7.154}$$

This expression shows that $f^{(2)}$ corresponds to scattering view as a two-step process.



Physical interpretation of the higher-order Born term $f^{(2)}(\mathbf{k}', \mathbf{k})$.

This scheme can obviously be continued to higher orders.

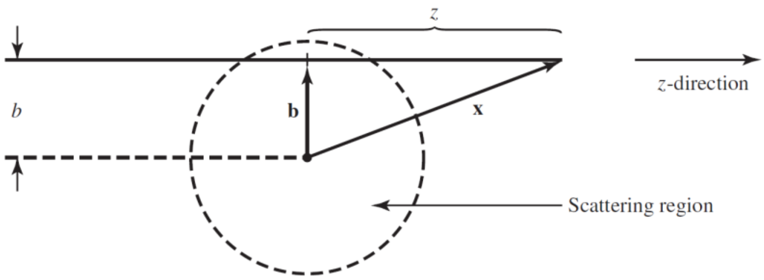
7.3.4 Eikonal Approximation

This approximation covers a situation in which $V(\mathbf{x})$ varies very little and $E \gg |V|$. The exact wave function $\psi^{(+)}$ can be replaced by the semiclassical wave function

$$\psi^{(+)} \sim \exp\left[iS(\mathbf{x})/\hbar\right]. \tag{7.155}$$

This leads to the Hamilton-Jacobi equation

$$\frac{(\nabla S)^2}{2m} + V = E = \frac{\hbar^2 k^2}{2m}. \tag{7.156}$$



Schematic diagram of eikonal approximation scattering where the classical straight-line trajectory is along the z-direction, $|\mathbf{x}| = r$, and $b = |\mathbf{b}|$ is the impact parameter.

For small deflection at high energy, it can be approximated that a straight-line path of the classical trajectory is satisfactory. Integrating Eq. (7.156), we have

$$\frac{S}{\hbar} = \int_{-\infty}^{z} \left[k^2 - \frac{2m}{\hbar^2} V\sqrt{b^2 + z'^2}\right]^{1/2} \mathrm{d}z' + \text{constant}. \tag{7.157}$$

The constant should be so chosen that

$$\frac{S}{\hbar} \to kz, \quad V \to 0. \tag{7.158}$$

To reproducing Eq. (7.155) in the zero-potential limit. Eq. (7.157) is then

$$\frac{S}{\hbar} = kz + \int_{-\infty}^{z}\left[\sqrt{k^2 - \frac{2m}{\hbar^2}V\sqrt{b^2+z'^2}} - k\right]\mathrm{d}z' \cong kz - \frac{m}{\hbar^2 k}\int_{-\infty}^{z} V\left(\sqrt{b^2+z'^2}\right)\mathrm{d}z', \quad (7.159)$$

where for $E \gg V$ we have used

$$\sqrt{k^2 - \frac{2m}{\hbar^2}V\sqrt{b^2+z'^2}} \sim k - \frac{mV}{\hbar^2 k} \quad (7.160)$$

at high energy $E = \hbar^2 k^2 / 2m$. So

$$\psi^{(+)}(\mathbf{x}) = \psi^{(+)}(\mathbf{b} + z\hat{\mathbf{z}}) \simeq \frac{1}{(2\pi)^{3/2}}\exp(ikz)\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{z} V\left(\sqrt{b^2+z'^2}\right)\mathrm{d}z'\right]. \quad (7.161)$$

According to Eq. (7.58), the approximate scattering amplitude is

$$\begin{aligned} f(\mathbf{k}',\mathbf{k}) &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int \mathrm{d}^3x' \exp(-i\mathbf{k}'\cdot\mathbf{x}')V\left(\sqrt{b^2+z'^2}\right)\exp(i\mathbf{k}\cdot\mathbf{x}') \\ &\times \exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{z'} V\left(\sqrt{b^2+z''^2}\right)\mathrm{d}z''\right] \end{aligned}. \quad (7.162)$$

Using

$$\mathrm{d}^3x = b\mathrm{d}b\mathrm{d}\phi_b dz' \quad (7.163)$$

and, for small deflection θ ($\mathbf{k} \perp \mathbf{b}$ and $(\mathbf{k}-\mathbf{k}')\cdot\hat{\mathbf{z}} \sim O(\theta^2)$,

$$(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}' = (\mathbf{k}-\mathbf{k}')\cdot(\mathbf{b}+z'\hat{\mathbf{z}}) \simeq -\mathbf{k}'\cdot\mathbf{b}, \quad (7.164)$$

along with

$$\mathbf{k}'\cdot\mathbf{b} = (k\sin\theta\hat{\mathbf{x}} + k\cos\theta\hat{\mathbf{z}})\cdot(b\cos\phi_b\hat{\mathbf{x}} + b\sin\phi_b\hat{\mathbf{y}}) \simeq kb\theta\cos\phi_b \quad (7.165)$$

by choosing scattering to be in the *xz*-plane, Eq. (7.162) becomes

$$\begin{aligned} f(\mathbf{k}',\mathbf{k}) &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int b\mathrm{d}b\int_0^{2\pi}\mathrm{d}\phi_b \exp(-ikb\theta\cos\phi_b) \\ &\times \int_{-\infty}^{\infty}\mathrm{d}zV\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{z} V\mathrm{d}z'\right] \end{aligned}. \quad (7.166)$$

Denote

$$\int_0^{2\pi}\mathrm{d}\phi_b \exp(-ikb\theta\cos\phi_b) = 2\pi J_0(kb\theta) \quad (7.167)$$

and noticing that

$$\int_{-\infty}^{\infty}\mathrm{d}zV\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{z} V\mathrm{d}z'\right] = i\frac{\hbar^2 k}{m}\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{z} V\mathrm{d}z'\right]_{z=-\infty}^{z=\infty}, \quad (7.168)$$

finally

$$f(\mathbf{k}',\mathbf{k}) = -ik\int_0^{\infty}\mathrm{d}bbJ_0(kb\theta)\left[\exp(2i\Delta(b)) - 1\right], \quad (7.169)$$

where

$$\Delta(b) = -\frac{m}{2k\hbar^2}\int_{-\infty}^{\infty} V\left(\sqrt{b^2+z^2}\right)\mathrm{d}z. \quad (7.170)$$

The eikonal approximation satisfies the optical theorem Eq. (7.60).

7.3.5 Patial Waves and the Eikonal Approximation

The eikonal approximation is valid at high energies $\lambda\!\!\!^{-} \ll R$, where R is the range of the scatterer, so many partial waves contribute and we may regard l as a continuous variable. We can make the semiclassical argument that

$$l = bk \tag{7.171}$$

and take

$$l_{\max} = kR\,. \tag{7.172}$$

For large l and small θ, we substitute in Eq. (7.105)

$$\begin{aligned}&\sum_{l}^{l_{\max}} \to k\int \mathrm{d}b\\ &P_l(\cos\theta) \simeq J_0(l\theta) = J_0(kb\theta)\\ &\delta_l \to \Delta(b)\big|_{b=l/k}\end{aligned} \tag{7.173}$$

to obtain

$$\begin{aligned}&f(\theta) \to k\int \mathrm{d}b\frac{2kb}{2ik}\left(\exp\left[2i\Delta(b)\right]-1\right)J_0(kb\theta)\\ &= -ik\int \mathrm{d}bbJ_0(kb\theta)\left(\exp\left[2i\Delta(b)\right]-1\right)\end{aligned}. \tag{7.174}$$

At high energies many l-values up to $l_{\max}$ contribute, so the total cross section is

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)\sin^2\delta_l\ . \tag{7.175}$$

By using Eq. (7.125), we obtain

$$\sin^2\delta_l = \frac{\tan^2\delta_l}{1+\tan^2\delta_l} = \frac{\left[j_l(kR)\right]^2}{\left[j_l(kR)\right]^2+\left[n_l(kR)\right]^2} \simeq \sin^2\left(kR-\frac{\pi l}{2}\right), \tag{7.176}$$

where we have

$$\begin{aligned}&j_l(kr) \sim \frac{1}{kr}\sin\left(kr-\frac{l\pi}{2}\right)\\ &n_l(kr) \sim -\frac{1}{kr}\cos\left(kr-\frac{l\pi}{2}\right)\end{aligned}. \tag{7.177}$$

Therefore, we have

$$\begin{aligned}&\sin^2\delta_l + \sin^2\delta_{l+1} = \sin^2\delta_l + \sin^2(\delta_l - \pi/2)\\ &= \sin^2\delta_l + \cos^2\delta_l = 1\end{aligned}. \tag{7.178}$$

Because so many l-values contribute to Eq. (7.175), we may replace $\sin^2\delta_l$ by its average value of 1/2 given by Eq. (7.178) to obtain

$$\delta_{\text{tot}} = \frac{4\pi}{k^2}(kR)^2\frac{1}{2} = 2\pi R^2\,, \tag{7.179}$$

which is not the geometric cross section πR^2 either!

The factor of 2 can be understood by splitting Eq. (7.105) into the reflection part f_{r} and the shadow part f_{s} behind the scatterer as

$$\begin{aligned} f(\theta) &= f_{\mathrm{r}}(\theta)+f_{\mathrm{s}}(\theta) \\ f_{\mathrm{r}}(\theta) &= \frac{1}{2ik}\sum_{l=0}^{l_{\max}}(2l+1)\exp(2i\delta_l)P_l(\cos\theta). \\ f_{\mathrm{s}}(\theta) &= \frac{i}{2k}\sum_{l=0}^{l_{\max}}(2l+1)P_l(\cos\theta) \end{aligned} \tag{7.180}$$

The contribution to the total cross section by $f_{\mathrm{r}}(\theta)$ is

$$\int\left|f_{\mathrm{r}}(\theta)\right|^2 \mathrm{d}\Omega = \frac{2\pi}{4k^2}\sum_{l=0}^{l_{\max}}\int_{-1}^{1}(2l+1)^2\left[P_l(\cos\theta)\right]^2 \mathrm{d}(\cos\theta) = \frac{\pi l_{\max}^2}{k^2} = \pi R^2 . \tag{7.181}$$

Using the small-angle approximation for P_l, we obtain

$$f_{\mathrm{s}} \simeq \frac{i}{2k}\sum(2l+1)J_0(l\theta) \simeq ik\int_0^R b\mathrm{d}bJ_0(kb\theta) = i\frac{R}{\theta}J_1(kR\theta). \tag{7.182}$$

Letting $\xi = kR\theta$ and $\mathrm{d}\xi/\xi = \mathrm{d}\theta/\theta$, we can evaluate

$$\int\left|f(\theta)_{\mathrm{s}}\right|^2 \mathrm{d}\Omega = 2\pi\int_{-1}^{1}\frac{R^2}{\theta^2}\left[J_1(kR\theta)\right]^2 \mathrm{d}(\cos\theta) \simeq 2\pi R^2\int_0^\infty \frac{\left[J_1(\xi)\right]^2}{\xi}\mathrm{d}\xi \simeq \pi R^2 . \tag{7.183}$$

Finally, because the phase of $f_{\mathrm{r}}(\theta)$ oscillates ($2\delta_{l+1} = 2\delta_l - \pi$), approximately averaging to zero, while $f_{\mathrm{s}}(\theta)$ is purely imaginary, the interference between them vanishes:

$$\mathrm{Re}\left(f_s^* f_{\mathrm{r}}\right) \simeq 0 . \tag{7.184}$$

Therefore, we can see

$$\sigma_{\mathrm{tot}} = \sigma_{\mathrm{r}} + \sigma_{\mathrm{s}} . \tag{7.185}$$

The optical theorem Eq. (7.60) can be verified by

$$\frac{4\pi}{k}\mathrm{Im}\, f(0) \simeq \frac{4\pi}{k}\mathrm{Im}\left[f_{\mathrm{s}}(0)\right] = \frac{4\pi}{k}\mathrm{Im}\left[\frac{i}{2k}\sum_{i=0}^{kR}(2l+1)P_l(1)\right] = 2\pi R^2 = \sigma_{\mathrm{tot}} . \tag{7.186}$$