The Optical Theorem

1. The probability currents

In the quantum theory of scattering, the optical theorem is a consequence of the conservation of probability. As usual, we define

$$\rho(\vec{\boldsymbol{x}},t) \equiv |\Psi(\vec{\boldsymbol{x}},t)|^2\,, \qquad\qquad \vec{\boldsymbol{j}}(\vec{\boldsymbol{x}},t) = -\frac{i\hbar}{2m}\left[\Psi^*(\vec{\boldsymbol{x}},t)\vec{\boldsymbol{\nabla}}\Psi(\vec{\boldsymbol{x}},t) - \Psi(\vec{\boldsymbol{x}},t)\vec{\boldsymbol{\nabla}}\Psi^*(\vec{\boldsymbol{x}},t)\right]\,. \tag{1}$$

The conservation of probability is expressed by

$$\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{j}} + \frac{\partial\rho}{\partial t} = 0\,.$$

For a stationary state solution, $\Psi(\vec{\boldsymbol{x}},t)$ is independent of time, in which case, $\partial\rho/\partial t = 0$. Hence, it follows that $\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{j}} = 0$. Integrating this equation over the volume of a sphere (centered at the origin) of radius $R \gg r_0$, where r_0 is the range of the potential, it follows that

$$\int_V \vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{j}}\,d^3x = \oint_S \vec{\boldsymbol{j}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,da = r^2\oint_S \vec{\boldsymbol{j}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,d\Omega = 0\,, \tag{2}$$

where S is the surface of a sphere of radius R centered at the origin.

In scattering theory, the asymptotic form for the wave function is a stationary state that represents the incoming plane wave an an outgoing (scattered) spherical wave,

$$\Psi_{\boldsymbol{k}}(\vec{\boldsymbol{x}}) = e^{i\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}} + f(\theta,\phi)\,\frac{e^{ikr}}{r}\,, \qquad\qquad \text{as } r\to\infty\,. \tag{3}$$

In spherical coordinates, we have,

$$\vec{\boldsymbol{\nabla}} = \hat{\boldsymbol{r}}\,\frac{\partial}{\partial r} + \mathcal{O}\left(\frac{1}{r}\right)\,.$$

Inserting eq. (3) into the definition of the probability current [eq. (1)], it follows that

$$\vec{\boldsymbol{j}} = \frac{\hbar}{m}\left[\vec{\boldsymbol{k}} + k\hat{\boldsymbol{r}}\,\frac{|f(\theta,\phi)|^2}{r^2}\right] + \vec{\boldsymbol{j}}_{\rm int}\,, \tag{4}$$

where

$$\vec{\boldsymbol{j}}_{\rm int} = -\frac{\hbar k}{2mr}\,(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\left[f(\theta,\phi)e^{-i(\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}-kr)} + f^*(\theta,\phi)e^{i(\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}-kr)}\right] \tag{5}$$

is the contribution to the probability current due to the interference between the incoming plane wave and the outgoing (scattered) spherical wave.

2. Evaluation of $\lim_{r\to\infty} e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}$

To compute the cross section, we need the asymptotic forms for the probability currents given in eqs. (4) and (5). In particular, we need to make sense of[1]

$$\lim_{r\to\infty} e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}\,, \qquad \text{where } r\equiv|\vec{\boldsymbol{x}}|\,. \tag{6}$$

Strictly speaking, the above limit does not exist. However, this limit does exist in the sense of distributions. This is not surprising, since plane waves are an idealization of the initial state of the scattering process. In reality, the initial state is more realistically represented by a wave packet with some spread of initial momenta $\hbar\vec{\boldsymbol{k}}$. Employing the plane wave simplifies the mathematical analysis, although with a price of dealing with certain quantities such as eq. (6) that must be carefully treated.

To evaluate the limit in eq. (6), we begin with the well-known expansion of the plane wave in terms of spherical waves,

$$e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}} = 4\pi\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr) Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}})\,, \tag{7}$$

where $Y_{\ell m}(\hat{\boldsymbol{r}})\equiv Y_{\ell m}(\theta_r,\phi_r)$ and $Y_{\ell m}(\hat{\boldsymbol{k}})\equiv Y_{\ell m}(\theta_k,\phi_k)$. That is, the unit vectors $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{k}}$ are specified by polar and azimuthal angles (θ_r,ϕ_r) and (θ_k,ϕ_k), respectively. Asymptotically, we have as $r\to\infty$,

$$j_\ell(kr) = \frac{\sin(kr-\frac{1}{2}\ell\pi)}{kr} + \mathcal{O}\left(\frac{1}{r^2}\right) = \frac{1}{kr}\left[\sin kr\cos(\tfrac{1}{2}\ell\pi) - \cos kr\sin(\tfrac{1}{2}\ell\pi)\right] + \mathcal{O}\left(\frac{1}{r^2}\right)\,.$$

Inserting this result into eq. (7) yields

$$\begin{aligned}\lim_{r\to\infty} e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}} &= 4\pi\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{i^\ell}{kr}\left[\sin kr\cos(\tfrac{1}{2}\ell\pi) - \cos kr\sin(\tfrac{1}{2}\ell\pi)\right]Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}}) \\ &= 4\pi\left\{\frac{\sin kr}{kr}\sum_{\ell\text{ even}}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}}) - \frac{i\cos kr}{kr}\sum_{\ell\text{ odd}}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}})\right\}\,, \end{aligned} \tag{8}$$

after using

$$\sin(\tfrac{1}{2}\ell\pi) = \begin{cases} i^{\ell-1}\,, & \text{for odd } \ell\,, \\ 0 & \text{for even } \ell\,, \end{cases} \qquad\qquad \cos(\tfrac{1}{2}\ell\pi) = \begin{cases} 0\,, & \text{for odd } \ell\,, \\ i^\ell & \text{for even } \ell\,. \end{cases}$$

To evaluate the sums in eq. (8), we consider the completeness relation,

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}}) = \delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\,, \tag{9}$$

[1]The limit $r\to\infty$ really means that we take the dimensionless quantity $kr\to\infty$.

where the delta function above means

$$\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})=\delta(\Omega_k-\Omega_r)=\delta(\cos\theta_k-\cos\theta_r)\delta(\phi_k-\phi_r)\,,$$

so that

$$\int d\Omega_k\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})=1\,.$$

Noting that

$$Y_{\ell m}(-\hat{\boldsymbol{r}})=Y_{\ell m}(\pi-\theta_r\,,\,\phi_r+\pi)=(-1)^\ell\,Y_{\ell m}(\theta_r,\phi_r)=(-1)^\ell\,Y_{\ell m}(\hat{\boldsymbol{r}})\,,$$

it follows that

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}(-1)^\ell\,Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}})=\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\,. \tag{10}$$

Adding and subtracting eqs. (9) and (10) then yields

$$\sum_{\ell\ \text{even}}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}})=\tfrac{1}{2}\left[\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})+\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\right]\,,$$

$$\sum_{\ell\ \text{odd}}\sum_{m=-\ell}^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{r}})=\tfrac{1}{2}\left[\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})-\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\right]\,.$$

Using the above results to evaluate eq. (8), we end up with

$$\lim_{r\to\infty}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}=\frac{2\pi i}{kr}\left[e^{-ikr}\,\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})-e^{ikr}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\right]\,. \tag{11}$$

That is, $\lim_{r\to\infty}e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}$ can be understood as a distribution (often called a generalized function) that can be expressed in terms of delta functions. Distributions acquire meaning when multiplied by a smooth function and integrated over an appropriate region. In principle, one can derive the entire asymptotic series for $e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}$ as $r\to\infty$ by employing the full asymptotic series for $j_\ell(kr)$ in eq. (7). Eq. (11) can also be viewed as a particular generalization of the Riemann-Lebesgue lemma.

3. Derivation of the Optical Theorem

We can now compute the large r behavior of eq. (5). Using eq. (11),

$$\lim_{r\to\infty}e^{i(\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}-kr)}=\frac{2\pi i}{kr}\left[e^{-2ikr}\,\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})-\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\right]\,.$$

Hence, it follows that

$$\lim_{r\to\infty}(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})e^{i(\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}-kr)}=-\frac{4\pi i}{kr}\,\hat{\boldsymbol{k}}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\,,$$

after employing the identities, $(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})=0$ and $(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})=2\hat{\boldsymbol{k}}\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})$.

Consequently,

$$\vec{\boldsymbol{j}}_{\rm int} = -\frac{\hbar k}{2mr}\,\frac{4\pi i}{kr}\,\hat{\boldsymbol{k}}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\,[f^*(\theta,\phi)-f(\theta,\phi)]$$
$$= -\frac{4\pi\hbar}{mr^2}\,\hat{\boldsymbol{k}}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}}){\rm Im}\,f(\theta,\phi)\,. \qquad (12)$$

The effect of the $\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})$ in eq. (12) is to set $\theta=0$ (the corresponding value of ϕ is irrelevant). Hence, eqs. (4) and (5) yield

$$\vec{\boldsymbol{j}} = \frac{\hbar k}{m}\left[\hat{\boldsymbol{k}}\left(1-\frac{4\pi}{kr^2}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\,{\rm Im}\,f(\theta=0)\right)+\frac{\hat{\boldsymbol{r}}}{r^2}\,|f(\theta,\phi)|^2\right]+\mathcal{O}\left(\frac{1}{r^3}\right)\,. \qquad (13)$$

Using eq. (2), we must evaluate the following integrals,

$$\int \hat{\boldsymbol{k}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,d\Omega = \int \cos\theta\,d\Omega = 0\,,$$

$$\int \hat{\boldsymbol{k}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})\,d\Omega = \hat{\boldsymbol{k}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\Big|_{\hat{\boldsymbol{r}}=\hat{\boldsymbol{k}}} = 1\,,$$

$$\int |f(\theta,\phi)|^2\,d\Omega = \sigma_T\,, \qquad (14)$$

where σ_T is the total cross-section for scattering.[2] Therefore, eqs. (2) and (13) yield

$$-\frac{4\pi}{k}\,{\rm Im}\,f(\theta=0)+\sigma_T=0\,,$$

which is the celebrated optical theorem,

$${\rm Im}\,f(\theta=0) = \frac{k}{4\pi}\sigma_T\,. \qquad (15)$$

The derivations presented in Sections 1–3 above were inspired by Askold M. Perelomov and Yakov B. Zel'dovich, *Quantum Mechanics: Selected Topics* (World Scientific Publishing Company, Singapore, 1998), Chapter 2.4.

4. Another derivation of the Optical Theorem

It is instructive to present a second proof of eq. (15) using the abstract formulation of scattering theory. In abstract scattering theory, the integral equation for scattering is represented by the Lippmann-Schwinger equation,

$$|\Psi^{(+)}\rangle = |\vec{\boldsymbol{k}}\rangle + \frac{1}{E-H_0+i\epsilon}\,V|\Psi^{(+)}\rangle\,, \qquad (16)$$

[2]Recall that the definition of the cross-section is $d\sigma = \vec{\boldsymbol{j}}_{\rm sc}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,r^2\,d\Omega/j_{\rm inc}$, where $\vec{\boldsymbol{j}}_{\rm sc}=\hbar k\hat{\boldsymbol{r}}|f(\theta,\phi)|^2/(mr^2)$ and $j_{\rm inc}=\hbar k/m$. It follows that $d\sigma/d\Omega = |f(\theta,\phi)|^2$.

where the $(+)$ superscript (which corresponds to the sign of the $i\epsilon$) indicates that the scattered wave corresponds to *outgoing* spherical waves, and H_0 is the free-particle Hamiltonian (in absence of the scattering potential V). The states $|\vec{\boldsymbol{k}}\rangle$ are eigenstates of H_0 with corresponding eigenvalues $E = \hbar^2 k^2/(2m)$. The transition operator T is then defined by

$$T|\vec{\boldsymbol{k}}\rangle = V|\Psi^{(+)}\rangle\,. \tag{17}$$

The scattering amplitude $f(\theta,\phi)$ is related to the matrix elements of the transition operator,

$$f(\theta,\phi) = -\frac{4\pi^2 m}{\hbar^2}\langle\vec{\boldsymbol{k}}\,'|T|\vec{\boldsymbol{k}}\rangle\,, \tag{18}$$

where (θ,ϕ) are the polar and azimuthal angles of the vector $\vec{\boldsymbol{k}}$ in a coordinate system in which $\vec{\boldsymbol{k}} = k\hat{\boldsymbol{z}}$. Setting $\vec{\boldsymbol{k}}\,' = \vec{\boldsymbol{k}}$ is equivalent to setting $\theta = 0$; thus the forward scattering amplitude is

$$f(\theta=0) = -\frac{4\pi^2 m}{\hbar^2}\langle\vec{\boldsymbol{k}}|T|\vec{\boldsymbol{k}}\rangle\,.$$

Using eqs. (16) and (17), it follows that

$$\langle\vec{\boldsymbol{k}}|T|\vec{\boldsymbol{k}}\rangle = \langle\vec{\boldsymbol{k}}|V|\Psi^{(+)}\rangle = \langle\Psi^{(+)}|V|\Psi^{(+)}\rangle - \langle\Psi^{(+)}|V\,\frac{1}{E-H_0-i\epsilon}\,V|\Psi^{(+)}\rangle\,. \tag{19}$$

We now employ the formal operator identity,

$$\frac{1}{E-H_0-i\epsilon} = \mathrm{P}\,\frac{1}{E-H_0} + i\pi\delta(E-H_0)\,, \tag{20}$$

where P is the principal value. Under the assumption that V is hermitian,

$$\mathrm{Im}\,\langle\Psi^{(+)}|V|\Psi^{(+)}\rangle = \mathrm{Im}\,\langle\Psi^{(+)}|V\,\frac{1}{E-H_0}\,V|\Psi^{(+)}\rangle = 0\,,$$

since the diagonal elements of hermitian operators are real. Hence, eqs. (17)–(20) yield

$$\mathrm{Im}\,\langle\vec{\boldsymbol{k}}|T|\vec{\boldsymbol{k}}\rangle = -\pi\langle\Psi^{(+)}|V\,\delta(E-H_0)\,V|\Psi^{(+)}\rangle = -\pi\langle\vec{\boldsymbol{k}}|T^\dagger\,\delta(E-H_0)\,T|\vec{\boldsymbol{k}}\rangle\,.$$

To evaluate the above matrix element, we insert a complete set of eigenstates of H_0. Then, when $\delta(E-H_0)$ acts on $|\vec{\boldsymbol{k}}\,'\rangle$, it yields the "eigenvalue" $\delta\big(E - \hbar^2 k'^2/(2m)\big)$. That is, the operator delta-function is replaced by a c-number delta-function. Hence,

$$\mathrm{Im}\,\langle\vec{\boldsymbol{k}}|T|\vec{\boldsymbol{k}}\rangle = -\pi\int d^3k'\,\langle\vec{\boldsymbol{k}}|T^\dagger|\vec{\boldsymbol{k}}\,'\rangle\langle\vec{\boldsymbol{k}}\,'|T|\vec{\boldsymbol{k}}\rangle\delta\left(E-\frac{\hbar^2 k'^2}{2m}\right)\,. \tag{21}$$

Since $k \equiv |\vec{\boldsymbol{k}}|$ and $k' \equiv |\vec{\boldsymbol{k}}\,'|$ are both positive, the following identity can be used,

$$\delta\left(E-\frac{\hbar^2 k'^2}{2m}\right) = \delta\left(\frac{\hbar^2}{2m}(k^2-k'^2)\right) = \frac{m}{\hbar^2 k}\left[\delta(k-k')-\delta(k+k')\right] = \frac{m}{\hbar^2 k}\delta(k-k')\,,$$

after noting that $\delta(k+k') = 0$ since its argument can never be zero. Thus, the integral given in eq. (21) can be evaluated by writing $d^3k' = k'^2 dk' d\Omega$ using the delta-function to perform the integration over k'. The end result is given by

$$\mathrm{Im}\,\langle\vec{\boldsymbol{k}}|T|\vec{\boldsymbol{k}}\rangle = -\frac{\pi m k}{\hbar^2}\int d\Omega|\langle\vec{\boldsymbol{k}}\,'|T|\vec{\boldsymbol{k}}\rangle|^2$$

Finally, using eqs. (14) and (18) we recover the optical theorem given by eq. (15).