The Remnant of a Shadow

Unitarity in scattering theory and the optical theorem; what is the cross-section of a black disc of radius *a*?

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In this Chapter we consider scattering a particle a off another particle, or target, b. The outcome may be 'elastic', by which is meant that the same pair of particles emerges in the out-going state, $a+b\to a+b$, or 'inelastic', which means everything else: $a+b\to anything\ different$. Examples of inelastic collisions are, (i)a neutron striking a nucleus and leaving it in an excited state; (ii)a neutron striking a nucleus and being absorbed, forming a new nucleus; (iii)two or more completely different particles being formed, e.g., $p+\pi^-\to K^0+\Lambda^0$. Virtually all our information about particle physics is obtained from scattering experiments, so theorems about cross sections are particularly important.

I used to think that the optical theorem was something magical. It relates the total cross section to the imaginary part of the elastic forward scattering amplitude, thus,

$$\sigma_{TOT} = \frac{4\pi}{k} \operatorname{Im} (f_{el}(\theta = 0))$$
 (1)

where k is related to the momentum of the scattered particle in the normal way, $p = \hbar k$. (From this point in this Chapter we shall adopt the particle physics convention of dropping factors of c and \hbar). But the scattering amplitude is related to the differential cross-section, and thence to the total cross-section via,

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2 \qquad \text{and} \qquad \sigma = \int \frac{d\sigma}{d\Omega} d\Omega \qquad (2)$$

The quantities in (2) can be understood as applying to either the elastic process or some inelastic process. However, (1) relates the *total*, elastic plus inelastic, cross-section ($\sigma_{TOT} = \sigma_{el} + \sigma_{in}$) to the *elastic* forward scattering amplitude.

What puzzled me was how there could be enough information in the forward scattering amplitude, $f_{el}(\theta=0)$, to determine the total cross section. This seemed strange because the total cross-section is an integral over the (absolute square of the) scattering amplitude at all angles, not just the forward direction, (2). Moreover, how could the forward elastic amplitude tell us anything about the inelastic channels, which are also included in the LHS of (1)?

But the optical theorem is not the remarkable dynamical constraint that I thought it was. Actually it is rather a prosaic result which follows simply from the conservation of probability, or unitarity. The key to demystifying the optical theorem is to recall what is meant by the scattering amplitude. In quantum mechanics, or field theory, the scattering process can represented by the S-matrix defined so that the probability amplitude for an initial state $|i\rangle$ producing a final state $|f\rangle$ is S_{fi} , the corresponding operator being such that,

$$S_{fi} = \langle f | S | i \rangle \tag{3}$$

Two things can happen: nothing or something. The former possibility, that the input state is unaffected by any interaction, is represented by the unit matrix, I. Consequently we write,

$$S = I + 2iT \tag{4}$$

The T-matrix in (4) is that part of the S-matrix which accounts for some change occurring. So the scattering amplitude, f, is proportional to T (or, rather, some matrix element thereof). Note that the factor of 2i in (4) is an arbitrary convention. More of normalisation issues later.

That the S-matrix must be unitary, $S^+S = I$, is easily established. The probability that the initial state $|i\rangle$ produces the final state $|f\rangle$ is $|S_{fi}|^2$. But any initial state must produce some final state, so we must have $\sum_{f} |S_{fi}|^2 = 1$, where the sum is over every possible final state. Hence,

$$\sum_{f} \left| S_{fi} \right|^{2} = \sum_{f} S_{fi}^{*} S_{fi} = \sum_{f} \left\langle i \left| S^{+} \right| f \right\rangle \left\langle f \left| S \right| i \right\rangle = \left\langle i \left| S^{+} S \right| i \right\rangle \equiv 1$$
 (5)

Because (5) must hold for an arbitrary input state, $|i\rangle$, it follows that all the diagonal elements of S^+S in some orthonormal basis are unity. However the same must be true for, say, the input state $(|i\rangle + |j\rangle)/\sqrt{2}$, where $|i\rangle$ and $|j\rangle$ are distinct orthonormal basis states. Then (5) gives,

$$\begin{split} \frac{1}{2} \Big(\! \left\langle i \right| + \left\langle j \right| \! \right) \! S^+ S \Big(\! \left| i \right\rangle + \left| j \right\rangle \! \Big) &\equiv 1 = \frac{1}{2} \Big[\! \left\langle i \right| \! S^+ S \big| i \right\rangle + \left\langle j \left| S^+ S \right| j \right\rangle + \left\langle i \left| S^+ S \right| j \right\rangle + \left\langle j \left| S^+ S \right| i \right\rangle \! \Big] \\ &= 1 + \frac{1}{2} \Big[\! \left\langle i \left| S^+ S \right| j \right\rangle + \left\langle j \left| S^+ S \right| i \right\rangle \! \Big] \end{split}$$

Hence,
$$\langle i|S^+S|j\rangle + \langle j|S^+S|i\rangle = 2\Re(\langle i|S^+S|j\rangle) = 0$$
 (6)

But we could have considered the input state $(i - i | j) / \sqrt{2}$ instead, in which case (6) would become $i \langle i | S^+ S | j \rangle - i \langle j | S^+ S | i \rangle = -2 \operatorname{Im}(\langle i | S^+ S | j \rangle) = 0$. So we conclude that $\langle i | S^+ S | j \rangle = 0$ for any pair of orthonormal states. Putting this together with (5) proves that the S-matrix is unitary,

$$S^+S = I \tag{7}$$

(Note that this is the same as saying that the Hermetian conjugate of S equals its inverse, $S^+ = S^{-1}$). Unitarity is simply the requirement for probability to be conserved – or perhaps consistency of interpretation may be a better way of expressing it.

Now if we substitute (4) into (7) we get,

$$(I + 2iT)^{+}(I + 2iT) = (I - 2iT^{+})(I + 2iT) = 1 + 4T^{+}T - 2i(T^{+} - T) = 1$$
Hence,
$$T^{+}T = \text{Im}(T)$$
(8)

One can already see the formal similarity between (1) and (8). Recalling that the scattering amplitudes are proportional to the corresponding matrix element of T. Hence, the scattering amplitude for an initial state $|i\rangle$ to produce a final state $|j\rangle$ is

 $f_{i \to j} \propto \langle j | T | i \rangle$. In particular, the forward elastic scattering amplitude, when the final state is the same as the initial state, is $f_{el}(\theta=0) \propto \langle el, \theta=0 | T | el, \theta=0 \rangle$. Taking this matrix element of (8) gives,

$$\langle el, \theta = 0 | T^{+}T | el, \theta = 0 \rangle = \sum_{j} \langle el, \theta = 0 | T^{+} | j \rangle \langle j | T | el, \theta = 0 \rangle = \operatorname{Im} \langle el, \theta = 0 | T | el, \theta = 0 \rangle$$
 (9)

Providing that the constant of proportionality in the relation $f_{i\to j} \propto \langle j|T|i\rangle$ is the same for all states then (9) implies,

$$\sum_{j} |f(el, \theta = 0 \to j)|^2 \propto \operatorname{Im}(f_{el}(\theta = 0))$$
(10)

But (2) shows that the summand in (10) is just the differential cross-section for some arbitrary elastic or inelastic collision, from the desired initial state. Summing over all possible states thus provides the total cross-section since the angular integration in (2) is subsumed in this sum, as is the sum over all possible inelastic channels (as well as elastic scattering). Consequently (10) is just the optical theorem, sans the coefficient of proportionality.

This demystifies the optical theorem. The important thing is that, due to (4), T, and hence f, are related to S-I, that is to the *change* in the initial state. The forward elastic scattering amplitude, $f_{el}(\theta=0)$, should not be confused with the total amplitude of the original state. It is the change in this amplitude. Clearly the only way in which either scattering away from the forward direction, or inelastic collisions, can occur is if the amplitude of the initial state reduces. So the total probability of all non-null transitions (σ_{TOT}) must be related to the change in the amplitude of the initial state, $f_{el}(\theta=0)$. That this relationship is linear in $f_{el}(\theta=0)$ results from the fact that the mechanism for the reduction in the forward elastic amplitude can only be interference between the unperturbed state and the scattered state, i.e., the two terms on the RHS of (4).

All that remains is to establish the constant of proportionality in (10). This is uniquely defined because the normalisation of the scattering amplitude is defined by its relation to the differential cross-section, (2). There is a multitude of different ways to derive the optical theorem. Schiff () does it via solutions to the Schrodinger equation, including the possibility of inelastic channels by considering complex potentials. Jackson () does it from the perspective of diffractive optics, in terms of the underlying electromagnetic fields. Gasiorowicz () does it from the particle physics perspective, illustrating the derivation by pion-nucleon scattering. Perl () does it in a more general fashion from the particle physics perspective. Many derivations use either the asymptotic form of a scattered wave or a partial wave expansion. The disadvantage of these derivations is that they may leave the reader with the impression that the optical theorem is reliant upon these mathematical descriptions being valid. But this is not so. Essentially we have all but established the theorem already, using unitarity alone, in the form (10). Establishing the factor of $4\pi/k$ is just a matter of getting the normalisations right. It is preferable, therefore, to employ a method which introduces no extra assumptions but rather emphasises that proper normalisation is the issue. It is also preferable to be explicitly relativistic (Lorentz covariant). This can be done easily enough, but is rather long winded since various standard formulae for the cross section and differential cross section need to be

derived. This derivation is sketched in the Appendix. Here we prefer a quicker way to the result, but restricted to non-relativistic, elastic scattering and at the expense of introducing a particular asymptotic form of the scattered wave. The Appendix shows that none of these restrictions is necessary.

For elastic scattering the asymptotic form of the wave equals the incoming plane wave plus the scattered wave which diminishes in amplitude as 1/r, thus,

As
$$r \to \infty$$
:
$$\psi = e^{i\bar{k}\cdot\bar{r}} + \frac{f_{el}(\theta,\phi)}{r}e^{ikr}$$
 (11)

The elastic nature of the scattering is reflected in the wavenumber, k, being unchanged in the scattered wave. Equ.(11) explicitly introduces the scattering amplitude, f, in its simplest form. It can be an arbitrary function of the scattering angle. The intensity at large r is thus,

$$\left|\psi\right|^{2} = 1 + \frac{\left|f_{el}\left(\theta,\phi\right)\right|^{2}}{r^{2}} + \frac{f_{el}\left(\theta,\phi\right)}{r}e^{i\left(kr - \bar{k}\cdot\bar{r}\right)} + \frac{f_{el}\left(\theta,\phi\right)^{*}}{r}e^{-i\left(kr - \bar{k}\cdot\bar{r}\right)}$$
(12)

If we integrate over a large sphere to get the total flux it must equal the incoming flux, i.e., $\int |\psi|^2 r^2 d\Omega = \int 1 \cdot r^2 d\Omega$, and hence we must have,

$$\int r^{2} \left\{ \frac{\left| f_{el} \left(\theta, \phi \right) \right|^{2}}{r^{2}} + \frac{f_{el} \left(\theta, \phi \right)}{r} e^{i \left(kr - \bar{k} \cdot \bar{r} \right)} + \frac{f_{el} \left(\theta, \phi \right)^{*}}{r} e^{-i \left(kr - \bar{k} \cdot \bar{r} \right)} \right\} d\Omega = 0$$
 (13)

But $|f_{el}(\theta, \phi)|^2$ is just the differential cross-section, (2), so the first term in (13) is just the total elastic cross section. Hence,

As
$$r \to \infty$$
:
$$\sigma = -\int r \left\{ f_{el}(\theta, \phi) e^{i(kr - \bar{k} \cdot \bar{r})} + f_{el}(\theta, \phi)^* e^{-i(kr - \bar{k} \cdot \bar{r})} \right\} d\Omega$$
 (14)

Or,
$$\sigma = -\int r \left\{ f_{el}(\theta, \phi) e^{ikr(1-\cos\theta)} + f_{el}(\theta, \phi)^* e^{-ikr(1-\cos\theta)} \right\} d\Omega$$
 (15)

Now because $r \to \infty$ the exponents in (15) will vary very rapidly for small changes of angle, resulting in integration to virtually zero at all angles other than very near the forward direction, $\theta = 0$. The method of stationary phase gives an exact result in the limit $r \to \infty$. It can be evaluated from first principles as follows. Consider integration over a small range of θ near 0 for which we can put $1 - \cos \theta \approx \theta^2 / 2$. We have,

$$\int f(\theta, \phi) e^{ikr(1-\cos\theta)} d\Omega \approx 2\pi f(0) \int_{0}^{\theta} e^{ikr\theta^{2}/2} d(\theta^{2}/2) = \pi \cdot \frac{2}{ikr} \left(e^{ikr\theta^{2}/2} - 1 \right) f(0)$$
(16)

But as we consider increasing values of the small angle θ , the first term in (16) rotates rapidly around the Argand plane and averages to zero. We can then put,

$$\int f(\theta, \phi) e^{ikr(1-\cos\theta)} d\Omega \to \frac{2\pi i}{kr} f(0)$$
(17)

So (15) becomes simply,

$$\sigma = -r \left\{ \frac{2\pi i}{kr} f_{el}(0) - \frac{2\pi i}{kr} f_{el}(0)^* \right\} = \frac{4\pi}{k} \operatorname{Im}(f_{el}(0))$$
 (18)

which is the optical theorem, (1), for the case of elastic scattering.

As noted already, the basis of the optical theorem is simply that any, and all, particles emerging other than in the original state in the forward direction must be at the expense of a reduction in the forward elastic flux. There is another consequence of this simple observation. Consider a perfect absorber of geometrical area A. What is its total cross section? We can readily see that $\sigma_{TOT} > A$ because, in addition to the absorption cross-section of A, there will also be diffraction around the edges of the object, resulting in elastic scattering at small angles. Now the total wave is $\psi = \psi_i + \psi_s$, where ψ_i is the incoming wave and ψ_s is the scattered wave. But immediately behind the opaque object there is shadow. Consequently in this region there must be perfect destructive interference between these two components of the total wave, $\psi_s = -\psi_i$. The shadow does not extend to infinity, however. Diffraction around the object obliterates the shadow after a distance of the order ka^2 , where a is the smallest linear dimension of the area A. This diffracted wave is the very ψ_s which causes the shadow. But since $\psi_s = -\psi_i$ over the area A immediately behind the object, the associated diffracted flux is equal to that absorbed. So there is an elastic cross section equal to the absorption cross section of A. The total cross section is therefore $\sigma_{TOT} = 2A$. For example a perfectly black disc of radius a has a cross section of $\sigma_{TOT} = 2\pi a^2$, not πa^2 which might naively have been expected. The elastically scattered flux of $A|\psi_i|^2$ is the diffracted wave near the forward direction, visible in principle at distances greater than $\sim ka^2$. Since this diffracted wave originates from the shadow and is visible beyond the shadow, it can be regarded as the remnant of the shadow.

This 'shadow scattering' has been discussed by Peierls () and Schiff (1954) though the phenomenon, like the optical theorem, was known within classical optics much earlier.

Appendix – Covariant Derivation Without Extra Assumptions

We start by noting that (4) is not the most appropriate definition of T for a continuum of plane wave states, since it is bound to contain a factor of $\delta^4(P_f-P_i)$ where P_i,P_f are the total 4-momenta of all the particles involved in the initial and final state respectively. The delta function expresses the conservation of energy and momentum. It is more appropriate to extract this factor from the definition of T. There is no universally agreed convention but one commonly used one is,

$$S_{fi} = I_{fi} + i(2\pi)^4 \delta^4 (P_f - P_i) T_{fi}$$
 (19)

We now need to find the equivalent of (8), the unitarity condition, with this normalisation of T, and also to express the cross-section in terms of this T so as to make contact with the scattering amplitude through (2). We shall assume scalar particles. No problems of principle arise if the particles have spin, but for simplicity we are not carrying through the spin indices.

We shall take plane wave states, labelled by their 4-momenta, to be normalised so that,

$$\langle p'|p\rangle = (2\pi)^3 2E\delta^3(\overline{p}' - \overline{p}) \tag{20}$$

where $E = p^0$. This corresponds to a density of states such that the momentum space integration measure is,

$$\frac{d^3p}{(2\pi)^3 2E} \tag{21}$$

These are consistent in the sense that integration of $|p'\rangle\langle p'|$ over all states using (13) as the integration measure yields the identity operator, as we expect, i.e.,

$$\int \frac{d^3 p'}{(2\pi)^3 2E'} |p'\rangle\langle p'|p\rangle = \int \frac{d^3 p'}{(2\pi)^3 2E'} |p'\rangle\langle 2\pi\rangle^3 2E\delta^3(\overline{p'} - \overline{p}) = |p\rangle$$
 (22)

Note that (12) and (13) are not completely arbitrary. It is required that both be Lorentz scalars, which the factor of E accomplishes. Those familiar with field theory will recognise (13) as the integration measure used to form the fields by integrating over plane wave states. I recall being misled into believing that this was an arbitrary normalisation convention. But clearly it is not since the denominator of E in (13) affects the energy dependence of calculated cross-sections in field theory. The integration measure (13) is motivated by the fact that the particle probability density for a scalar field obeying the Klein-Gordon equation is $i\Phi^+\ddot{\partial}_0\Phi$ and the time derivative brings down the factor of E.

In view of (13), the unitarity condition expressed in terms of the T-matrix, (8), becomes.

$$(2\pi)^4 \sum_{f} \int_{k=1}^{N_f} \frac{d^3 p_k}{(2\pi)^3 2E_k} T_{jf}^+ T_{fi} \delta^4 (P_f - P_i) = i (T_{ji}^+ - T_{ji})$$
 (23)

In (15) the sum variable, f, denotes the different possible products of the collision whilst the integration is over the momenta of the N_f particles involved. For the purposes of establishing the optical theorem we need (15) only for the case that i = j = the elastic forward scattered state. Hence,

$$(2\pi)^4 \sum_{f} \int_{k=1}^{N_f} \frac{d^3 p_k}{(2\pi)^3 2E_k} |T_{fi}|^2 \delta^4 (P_f - P_i) = 2 \operatorname{Im}(T_{el}(\theta = 0))$$
 (24)

The derivation of the expression for the total cross section in terms of the T-matrix can be found in particle physics or field theory texts, such as Perl (), Mandl and Shaw (), or Martin and ? (). The starting point is the probability of the initial state becoming an arbitrary final state different from the initial state, which is obtained by summing over all final states using the integration measure, (13), which gives,

Probability of all outcomes =
$$\sum_{f} \int_{k=1}^{N_f} \frac{d^3 p_k}{(2\pi)^3 2E_k} S_{if}^+ S_{fi}$$
 (25)

Using (11), which becomes $S_{fi} = i(2\pi)^4 \delta^4 (P_f - P_i) T_{fi}$ for $f \neq i$, (17) can be re-written in terms of T. This involves potentially problematical products of delta functions, but these can pragmatically be interpreted by using $\delta^4(0) \rightarrow VT/(2\pi)^4$, where V is the normalisation volume for the plane waves and T is the period of time for which the incoming wave persists. Both these quantities cancel when forming the cross section,

since the cross section is defined in terms of the transitions per unit time and per target particle, and the latter is proportional to the volume. From (12) the number of target particles per unit volume in proportional to $E_b = m_b c^2$, the energy of the particle b, taken as the stationary target. The incoming flux of the particles of type a is thus $E_a v_a$, where v_a is their velocity. Hence (17) must be divided by a term proportional to $E_a E_b v_a$ to get the cross section in the laboratory frame. By noting that the Lorentz invariant quantity $\sqrt{(P_a \cdot P_b)^2 - m_a^2 m_b^2}$, where P_a, P_b are the 4-momenta, reduces to $E_a E_b v_a$ in the lab frame, the corresponding quantity in the centre-of-mass frame is seen to be $p^*(E_a^* + E_b^*)$, where the asterisks represent the com frame and p^* is the magnitude of one of the particle 3-momenta in this frame. Putting all these things together, and keeping track of the numerical factors, yields the total cross section for the initial state i is,

$$\sigma_{TOT} = \frac{(2\pi)^4}{4p^* (E_a^* + E_b^*)} \sum_f \int_{k=1}^{N_f} \frac{d^3 p_k}{(2\pi)^3 2E_k} |T_{fi}|^2 \delta^4 (P_f - P_i)$$
 (26)

But (18) is the same as the LHS of (16) apart from the denominator of $4p^*(E_a^* + E_b^*)$, so (16) becomes,

$$\sigma_{TOT} = \frac{2\operatorname{Im}(T_{el}(\theta=0))}{4p^*(E_a^* + E_b^*)}$$
(27)

The final relation that we need is that between T and f for elastic scattering in the com frame,

$$f_{el} = \frac{T_{el}}{8\pi (E_a^* + E_b^*)} \tag{28}$$

The proof of this follows from deriving the differential cross section from (18) and using (2). Details can be found in texts such as cited above. Substituting (20) into (19) final gives the optical theorem complete with its correct factor of proportionality,

$$\sigma_{TOT} = \frac{4\pi}{p^*} \operatorname{Im} \left(f_{el} \left(\theta = 0 \right) \right) \tag{29}$$

This is exactly as (1), but we now see that it is the commomentum which must be used, p^* .

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