

XIII

Scattering from inhomogeneous media

The term scattering covers a broad range of phenomena associated with the interaction of waves or particles with material media. In this chapter we will restrict ourselves to circumstances where the response of the medium to the incident wave is linear and can be described by macroscopic parameters such as the dielectric constant or, equivalently, by the refractive index or the dielectric susceptibility. We will also assume that the response is time-independent, i.e. that on a macroscopic level the physical properties of the medium do not change in the course of time. One then speaks of static scattering.

13.1 Elements of the scalar theory of scattering

13.1.1 Derivation of the basic integral equation

We consider a monochromatic electromagnetic field with time dependence $\exp(-i\omega t)$ (not explicitly shown in the subsequent analysis), incident on a linear, isotropic, nonmagnetic medium occupying a finite domain V (Fig. 13.1). Assuming that there are no sources in V , the space-dependent part of the complex electric field will satisfy the following equation which follows at once from §1.2 (5), specialized to a monochromatic wavefield:

$$\nabla^2 \mathbf{E}(\mathbf{r}, \omega) + k^2 \varepsilon(\mathbf{r}, \omega) \mathbf{E}(\mathbf{r}, \omega) + \text{grad}[\mathbf{E}(\mathbf{r}, \omega) \cdot \text{grad} \ln \varepsilon(\mathbf{r}, \omega)] = 0, \quad (1)$$

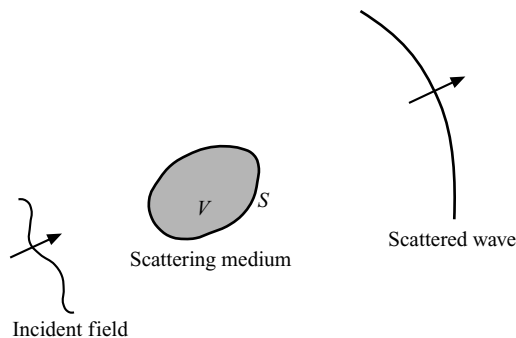


Fig. 13.1 Illustrating the notation relating to scattering on a medium occupying a volume V , bounded by a closed surface S .

with

$$k = \frac{\omega}{c}. \quad (2)$$

We note that the last term on the left of (1) couples the Cartesian components of the electric field. For this reason the treatment of scattering based on this equation is rather complicated. The equation can be simplified if we assume that the dielectric ‘constant’ $\varepsilon(\mathbf{r})$ varies so slowly with position that it is effectively constant over distances of the order of the wavelength $\lambda = 2\pi/k = 2\pi c/\omega$. Under these circumstances the last term on the left-hand side of (1) may be neglected. We then obtain the equation

$$\nabla^2 \mathbf{E}(\mathbf{r}, \omega) + k^2 n^2(\mathbf{r}, \omega) \mathbf{E}(\mathbf{r}, \omega) = 0, \quad (3)$$

where we have used the Maxwell formula $\varepsilon(\mathbf{r}, \omega) = n^2(\mathbf{r}, \omega)$, $n(\mathbf{r}, \omega)$ denoting the refractive index of the medium. We note that unlike in (1), the Cartesian components of $\mathbf{E}(\mathbf{r}, \omega)$ in (3) are no longer coupled and hence the implications of (3) are easier to analyse. In fact, a good insight into the general behaviour of the scattered field may be obtained by studying the behaviour of the solution of equation (3) for a single Cartesian component of $\mathbf{E}(\mathbf{r}, \omega)$. Denoting the component by $U(\mathbf{r}, \omega)$ we obtain the following scalar equation, which we will take as a starting point for our analysis of the scattered field:

$$\nabla^2 U(\mathbf{r}, \omega) + k^2 n^2(\mathbf{r}, \omega) U(\mathbf{r}, \omega) = 0. \quad (4)$$

Later, in §13.6, we will go beyond the scalar approximation and we will discuss scattering within the framework of the full electromagnetic theory.

It will be convenient to re-write (4) in the form

$$\nabla^2 U(\mathbf{r}, \omega) + k^2 U(\mathbf{r}, \omega) = -4\pi F(\mathbf{r}, \omega) U(\mathbf{r}, \omega), \quad (5)$$

where

$$F(\mathbf{r}, \omega) = \frac{1}{4\pi} k^2 [n^2(\mathbf{r}, \omega) - 1]. \quad (6)$$

The function $F(\mathbf{r}, \omega)$ is usually called *the scattering potential* of the medium, in analogy with the terminology used in the quantum theory of potential scattering, which is governed by an equation that is mathematically equivalent to (5), namely the time-independent Schrödinger equation for nonrelativistic particles.*

Let us express $U(\mathbf{r}, \omega)$ as the sum of the incident field, $U^{(i)}(\mathbf{r}, \omega)$ and of the scattered field $U^{(s)}(\mathbf{r}, \omega)$, [which may be regarded as defined by (7)],

$$U(\mathbf{r}, \omega) = U^{(i)}(\mathbf{r}, \omega) + U^{(s)}(\mathbf{r}, \omega). \quad (7)$$

The incident field is usually a plane wave. Such a field satisfies the Helmholtz equation

$$(\nabla^2 + k^2) U^{(i)}(\mathbf{r}, \omega) = 0 \quad (8)$$

throughout the whole space. On substituting from (7) into (5) and using (8) we see that the scattered field satisfies the equation

* See, for example, P. Roman, *Advanced Quantum Theory* (Reading, MA, Addison-Wesley, 1965), Chapt. III.

$$(\nabla^2 + k^2)U^{(s)}(\mathbf{r}, \omega) = -4\pi F(\mathbf{r}, \omega)U(\mathbf{r}, \omega). \quad (9)$$

Some of the consequences of this differential equation can best be studied by converting it to an integral equation, which can be done as follows:

Let $G(\mathbf{r} - \mathbf{r}')$ be a Green's function of the Helmholtz operator, i.e. a solution of the equation

$$(\nabla^2 + k^2)G(\mathbf{r} - \mathbf{r}', \omega) = -4\pi\delta^{(3)}(\mathbf{r} - \mathbf{r}'), \quad (10)$$

where $\delta^{(3)}(\mathbf{r} - \mathbf{r}')$ is the three-dimensional Dirac delta function. Let us multiply (9) by $G(\mathbf{r} - \mathbf{r}', \omega)$, (10) by $U^{(s)}(\mathbf{r}, \omega)$ and subtract the resulting equations from each other. This gives

$$\begin{aligned} U^{(s)}(\mathbf{r}, \omega)\nabla^2 G(\mathbf{r} - \mathbf{r}', \omega) - G(\mathbf{r} - \mathbf{r}', \omega)\nabla^2 U^{(s)}(\mathbf{r}, \omega) \\ = 4\pi F(\mathbf{r}, \omega)U(\mathbf{r}, \omega)G(\mathbf{r} - \mathbf{r}', \omega) - 4\pi U^{(s)}(\mathbf{r}, \omega)\delta^{(3)}(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (11)$$

Let us interchange \mathbf{r} and \mathbf{r}' and assume that the Green's function is symmetric, i.e. that $G(\mathbf{r} - \mathbf{r}', \omega) = G(\mathbf{r}' - \mathbf{r}, \omega)$. Next we integrate both sides of (11) with respect to \mathbf{r}' throughout a volume V_R , bounded by a large sphere S_R of radius R , centered on the origin O in the region of the scatterer and containing the scatterer in its interior (see Fig. 13.2). If we convert the volume integral on the left into a surface integral by the application of Green's theorem we obtain, after trivial manipulations, the formula

$$\begin{aligned} U^{(s)}(\mathbf{r}, \omega) = \int_V F(\mathbf{r}', \omega)U(\mathbf{r}', \omega)G(\mathbf{r} - \mathbf{r}', \omega) d^3 r' \\ - \frac{1}{4\pi} \int_{S_R} \left[U^{(s)}(\mathbf{r}', \omega) \frac{\partial G(\mathbf{r} - \mathbf{r}', \omega)}{\partial n'} - G(\mathbf{r} - \mathbf{r}', \omega) \frac{\partial U^{(s)}(\mathbf{r}', \omega)}{\partial n'} \right] dS_R, \end{aligned} \quad (12)$$

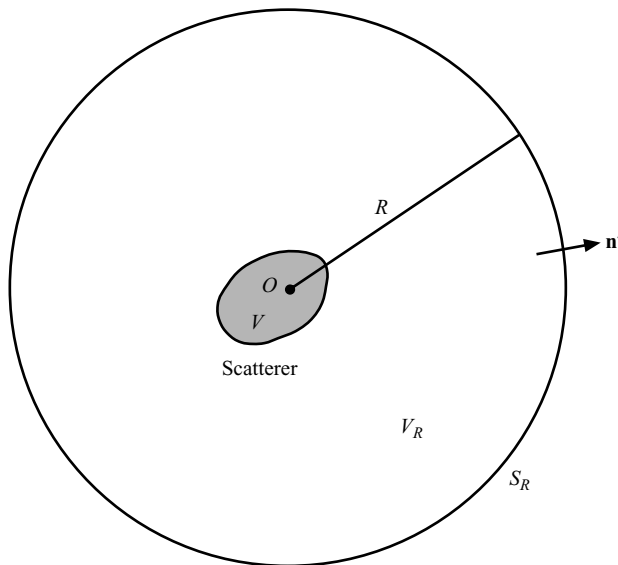


Fig. 13.2 Illustrating the notation relating to the derivation of (12).

where $\partial/\partial n'$ denotes differentiation along the outward normal \mathbf{n}' to S_R . The first integral on the right of (12) is taken only over the scattering volume V rather than over the whole volume V_R of the large sphere, because the scattering potential F vanishes throughout the exterior of V , as is evident from the definition (6).

So far we have not chosen any particular Green's function, i.e. any particular solution of (10). We have only assumed that it is symmetric. We will now make the choice

$$G(\mathbf{r} - \mathbf{r}', \omega) = \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}, \quad (13)$$

often called the *outgoing free-space Green's function* of the Helmholtz operator. It seems plausible that sufficiently far away from the scatterer, the scattered field $U^{(s)}(\mathbf{r}, \omega)$ will also behave as an outgoing spherical wave, a property which is usually postulated. Under these circumstances one would expect that in the limit as $R \rightarrow \infty$, the surface integral on the right of (12) will not contribute to the total field.* Hence we will omit it and (12) then reduces to

$$U^{(s)}(\mathbf{r}, \omega) = \int_V F(\mathbf{r}', \omega) U(\mathbf{r}', \omega) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} d^3 r'. \quad (14)$$

Suppose that the field incident on the scatterer is a monochromatic plane wave of unit amplitude and frequency ω , propagating in the direction specified by a real unit vector \mathbf{s}_0 . The time-independent part of the incident field is then given by the expression

$$U^{(i)}(\mathbf{r}, \omega) = e^{iks_0 \cdot \mathbf{r}}, \quad (15)$$

and it follows from (7) and (14) that

$$U(\mathbf{r}, \omega) = e^{iks_0 \cdot \mathbf{r}} + \int_V F(\mathbf{r}', \omega) U(\mathbf{r}', \omega) \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} d^3 r'. \quad (16)$$

Eq. (16) is the basic equation for determining the total field $U(\mathbf{r}, \omega)$ (incident + scattered) and is called the *integral equation of potential scattering*. It should be noted, however, that it is only an integral equation for the total field $U(\mathbf{r}, \omega)$ at points within the scattering volume V . Once the solution throughout V is known, the solution at points exterior to V can be obtained by substituting the solution to the 'interior' problem into the integrand of (16).

Unlike the differential equation (9), any solution of the integral equation (16) has necessarily the correct (outgoing) behaviour far away from the scatterer, as we will now verify by direct calculations.

Let Q be a typical point in the scattering volume V and P a point far away from it. Further let \mathbf{r}' be the position vector of Q and $\mathbf{r} = r\mathbf{s}$, ($s^2 = 1$), be the position vector of P and let N be the foot of the perpendicular dropped from Q onto the line OP (see Fig. 13.3). Then evidently, when r is large enough,

$$|\mathbf{r} - \mathbf{r}'| \sim r - \mathbf{s} \cdot \mathbf{r}' \quad (17)$$

* For a rigorous proof of this statement see B. B. Baker and E. T. Copson, *The Mathematical Theory of Huygens' Principle* (Oxford, Clarendon Press, 2nd edition, 1950), p. 24–25.

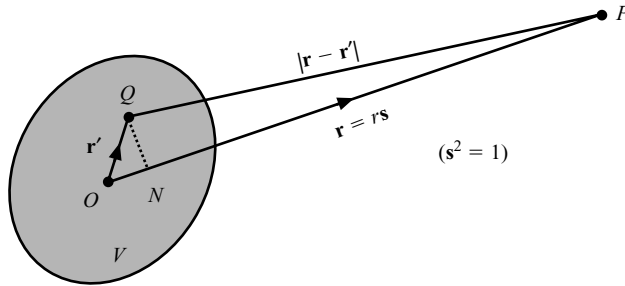


Fig. 13.3 Illustrating the notation relating to the approximation (17).

and

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \sim \frac{e^{ikr}}{r} e^{-iks \cdot \mathbf{r}'} \quad (18)$$

On using the approximation (18) in the integral in (16) we see that

$$U(r\mathbf{s}, \omega) \sim e^{iks_0 \cdot \mathbf{r}} + U^{(s)}(r\mathbf{s}, \omega), \quad (19)$$

where

$$U^{(s)}(r\mathbf{s}, \omega) = f(\mathbf{s}, \mathbf{s}_0; \omega) \frac{e^{ikr}}{r} \quad (20)$$

and

$$f(\mathbf{s}, \mathbf{s}_0; \omega) = \int_V F(\mathbf{r}', \omega) U(\mathbf{r}', \omega) e^{-iks \cdot \mathbf{r}'} d^3 r'. \quad (21)$$

More refined mathematical analysis shows that the expression on the right of (19), together with (20) and (21), is the asymptotic approximation for the total field $U(r\mathbf{s}, \omega)$ as $kr \rightarrow \infty$, with the direction \mathbf{s} being kept fixed. Formula (20) confirms that far away from the scatterer the scattered field $U^{(s)}(r\mathbf{s}, \omega)$ indeed behaves as an outgoing spherical wave, as expected. The function $f(\mathbf{s}, \mathbf{s}_0; \omega)$ is called the *scattering amplitude* and plays an important role in scattering theory.

13.1.2 The first-order Born approximation

In most situations of practical interest it is not possible to obtain solutions of the integral equation of potential scattering in a closed form. One must, therefore, try to solve it by some approximate technique. The most commonly used one is a method of perturbation, in which the successive terms in the perturbation expansion are obtained by iteration from the previous ones, provided that the medium scatters rather weakly. We will first discuss the lowest-order approximation which has many useful consequences and which provides a rough insight into various features of scattering. We will briefly consider the higher-order terms in §13.1.4.

From expression (6) for the scattering potential it is clear that a medium will scatter weakly if its refractive index differs only slightly from unity. Under these circum-

stances it is plausible to assume that one will obtain a good approximation to the total field U if the term $U = U^{(i)} + U^{(s)}$ under the integral in (16) is replaced by $U^{(i)}$. One then obtains as a first approximation to the solution of the integral equation of scattering, the expression (from now on we no longer display the dependence of the various quantities on the frequency ω)

$$U(\mathbf{r}) \approx U_1(\mathbf{r}) \equiv e^{ik\mathbf{s}_0 \cdot \mathbf{r}} + \int_V F(\mathbf{r}') e^{ik\mathbf{s}_0 \cdot \mathbf{r}'} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r'. \quad (22)$$

This approximate solution is generally referred to as the Born approximation or, more precisely, the *first-order Born approximation* (or just the first Born approximation).^{*} We will now discuss some of its consequences.

Frequently one makes measurements far away from the scatterer. One may readily define from (22) the behaviour of the far field. For this purpose we substitute for the spherical wave term in (22) the approximation (18) and find that (see Fig. 13.3)

$$U_1(r\mathbf{s}) \sim e^{ik(\mathbf{s}_0 \cdot \mathbf{r})} + f_1(\mathbf{s}, \mathbf{s}_0) \frac{e^{ikr}}{r}, \quad (\mathbf{s}_0^2 = 1), \quad (23)$$

as $kr \rightarrow \infty$ (\mathbf{s} fixed), where

$$f_1(\mathbf{s}, \mathbf{s}_0) = \int F(\mathbf{r}') e^{-ik(\mathbf{s}-\mathbf{s}_0) \cdot \mathbf{r}'} d^3 r'. \quad (24)$$

The expression (24) for the scattering amplitude $f_1(\mathbf{s}, \mathbf{s}_0)$ has important physical implications. To see this we first introduce the Fourier transform of the scattering potential,

$$\tilde{F}(\mathbf{K}) = \int F(\mathbf{r}') e^{-i\mathbf{K} \cdot \mathbf{r}'} d^3 r'. \quad (25)$$

Eq. (24) evidently implies that

$$f_1(\mathbf{s}, \mathbf{s}_0) = \tilde{F}[k(\mathbf{s} - \mathbf{s}_0)], \quad (26)$$

expressing a very basic result. It implies that *within the accuracy of the first-order Born approximation, the (generally complex) amplitude of the scattered wave (more precisely, the scattering amplitude) in the far zone of the scatterer, in the direction specified by the unit vector \mathbf{s} , depends entirely on one and only one Fourier component of the scattering potential, namely the one labelled by the vector[†]*

$$\mathbf{K} = k(\mathbf{s} - \mathbf{s}_0). \quad (27)$$

The simple formula (27) has immediate bearing on the problem of inverse scattering, i.e. the problem of obtaining information about an object from measurements of the field scattered by it. This formula shows that if a plane wave is incident on the scatterer in direction \mathbf{s}_0 and the scattered field is measured in direction \mathbf{s} , one can at

^{*} It is the first term in the perturbation expansion derived in the context of quantum mechanical collision theory by M. Born in *Z. Physik*, **38** (1926), 803.

[†] Formula (27) is the classical analogue of the so-called momentum transfer equation $\Delta \mathbf{p} = \mathbf{p} - \mathbf{p}_0$ in the quantum theory of elastic scattering, with \mathbf{p}_0 and \mathbf{p} representing the momentum of a particle before and after collision. Formally the momentum transfer equation may be deduced from (27) by using the Einstein–de Broglie relations $\mathbf{p}_0 = \hbar k\mathbf{s}_0$, $\mathbf{p} = \hbar k\mathbf{s}$, where \hbar is Planck's constant divided by 2π .

once determine from the measurement one Fourier component of the scattering potential: namely the one labelled by the spatial frequency vector (vector in \mathbf{K} -space) given by (27). Let us examine the totality of all the Fourier components of the scattering potential that can be deduced from such experiments. This can be done most elegantly by means of the following geometrical construction:

Suppose first that the object is illuminated in a direction \mathbf{s}_0 and that the complex amplitude of the scattered field is measured in the far zone in all possible directions \mathbf{s} . From such measurements one can obtain, according to (26) and (25), all those Fourier components $\tilde{F}(\mathbf{K})$ of the scattering potential $F(\mathbf{r})$ which are labelled by \mathbf{K} -vectors whose end points lie on a sphere σ_1 , of radius $k = \omega/c = 2\pi/\lambda$, centred on the point $-\mathbf{k}s_0$, λ being the wavelength associated with frequency ω . We will refer to this sphere as *Ewald's sphere of reflection* [see Fig. 13.4(a)], by analogy with the corresponding term used in the theory of X-ray diffraction by crystals, where the potential is a periodic function of position (briefly discussed in §13.1.3).

Next let us suppose that the object is illuminated in a different direction of incidence and that the scattered field is again measured in the far zone in all possible directions \mathbf{s} . From such measurements one obtains those Fourier components of the scattering potential which are labelled by \mathbf{K} -vectors whose end points lie on another Ewald sphere of reflection, σ_2 say [see Fig. 13.4(b)]. If one continues this procedure, for all possible directions of incidence \mathbf{s}_0 , one can determine all those Fourier components of the scattering potential which are labelled by \mathbf{K} -vectors whose end points fill the domain covered by the Ewald spheres of reflection associated with all possible

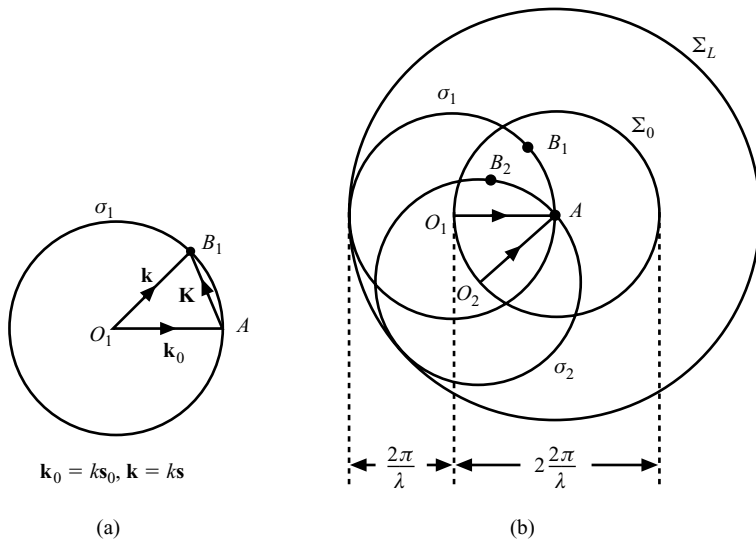


Fig. 13.4 (a) Ewald's sphere of reflection σ_1 , associated with the incident wave-vector $\mathbf{k}_0 = k\mathbf{s}_0 = \overrightarrow{O_1A}$. It is the locus of the end points of the vector $\mathbf{K} = \mathbf{k} - \mathbf{k}_0 = \overrightarrow{AB_1}$, with $\mathbf{k} = k\mathbf{s}$ representing the wave-vectors of the field scattered in all possible directions \mathbf{s} . (b) Ewald's limiting sphere Σ_L . It is the envelope of the spheres of reflections $\sigma_1, \sigma_2, \dots$, associated with all possible wave vectors $\overrightarrow{O_1A}, \overrightarrow{O_2A}, \dots$, of the incident fields. Σ_0 represents the sphere generated by the centers O_1, O_2, \dots , of the spheres of reflection associated with all possible directions of incidence.

directions of incidence. This domain is the interior of a sphere Σ_L of radius $2k = 4\pi/\lambda$, which may be called the *Ewald limiting sphere*.*

It follows from the preceding discussion that if one were to measure the scattered field in the far zone for all possible directions of incidence and all possible directions of scattering one could determine all those Fourier components $\tilde{F}(\mathbf{K})$ of the scattering potential labelled by \mathbf{K} -vectors of magnitude

$$|\mathbf{K}| \leq 2k = 4\pi/\lambda. \quad (28)$$

One could then synthesize all these Fourier components to obtain the approximation

$$F_{LP}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int_{|\mathbf{K}| \leq 2k} \tilde{F}(\mathbf{K}) e^{i\mathbf{K}\cdot\mathbf{r}} d^3 K, \quad (29)$$

called the *low-pass filtered approximation* to the scattering potential. The scattering potential itself contains all the Fourier components, being given in the inverse of (25), viz.

$$F(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \tilde{F}(\mathbf{K}) e^{i\mathbf{K}\cdot\mathbf{r}} d^3 K, \quad (30)$$

where the integration extends over the whole \mathbf{K} -space. Because the preceding analysis is based on the scalar approximation it was implicitly assumed that the scattering potential does not vary appreciably over distances of the order of the wavelength. Under these circumstances the low-pass filtered version of the scattering potential may be expected to be a good approximation to the true scattering potential.

The significance of the inequality (28) becomes somewhat more apparent by expressing it in terms of the spatial periods Δx , Δy , Δz of the scattering potential, defined by the formulae

$$\Delta x = \frac{2\pi}{|K_x|}, \quad \Delta y = \frac{2\pi}{|K_y|}, \quad \Delta z = \frac{2\pi}{|K_z|}, \quad (31)$$

where K_x , K_y , K_z are the Cartesian components of the vector \mathbf{K} . In terms of the spatial periods, the inequality (28) may be expressed as

$$\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2} \leq \left(\frac{2}{\lambda}\right)^2. \quad (32)$$

To obtain some indication of the implications of this inequality, let us consider its one-dimensional version, by formally letting $\Delta y \rightarrow \infty$, $\Delta z \rightarrow \infty$. The inequality then reduces to

$$\Delta x \geq \lambda/2. \quad (33)$$

This inequality indicates that measurements of the scattered field in the far zone would at best provide information about the structure of the scatterer down to details of the order of half a wavelength. There is no such simple interpretation of inequality (32) for the three-dimensional case but one can expect, roughly speaking, the low-pass

* The Ewald sphere of reflection and the Ewald limiting sphere were introduced in connection with the concept of the reciprocal lattice in classic investigations concerning the determination of the structure of crystals from X-ray diffraction measurements. (P. P. Ewald, *Phys. Z.*, **14** (1913), 465; J. D. Bernal, *Proc. Roy. Soc. A*, **113** (1927), 117.)

filtered approximation given by (29) to contain information about details of the object with resolution limit of the order of the wavelength.

The question of acquiring information about details smaller than about a wavelength or, more precisely, about the high spatial frequency components, whose representative \mathbf{K} -vectors have end points which lie outside the Ewald limiting sphere ($|\mathbf{K}| > 4\pi/\lambda$) has been studied by many authors in the context of the general theory of super-resolution and extrapolation.* The possibility of extracting such information from the low spatial frequency data is a consequence of the multi-dimensional form of the so-called Plancherel–Polya theorem.† In its one-dimensional form the theorem asserts that the Fourier transform $\tilde{f}(K)$ of a function $f(x)$ of finite support (i.e. a function which vanishes identically outside a finite x range) is the boundary value on the real K -axis of an entire analytic function of a complex K variable.‡ Hence, in principle, as a consequence of the three-dimensional version of this theorem, $\tilde{F}(\mathbf{K})$ can be analytically continued beyond the Ewald limiting sphere in \mathbf{K} -space. However, in practice only a very modest range of extrapolation is achievable because of effects of noise and instabilities.

13.1.3 Scattering from periodic potentials

We will illustrate the preceding analysis by considering scattering from periodic potentials.

Consider a weakly scattering object occupying a domain V which has the form of a rectangular parallelepiped

$$-\frac{1}{2}A \leq x \leq \frac{1}{2}A, \quad -\frac{1}{2}B \leq y \leq \frac{1}{2}B, \quad -\frac{1}{2}C \leq z \leq \frac{1}{2}C. \quad (34)$$

We assume that the scattering potential $F(x, y, z)$ of the object is periodic in the three axial directions, with periods $\Delta x = a$, $\Delta y = b$, $\Delta z = c$. We may then expand the scattering potential in a triple Fourier series

$$\left. \begin{aligned} F(x, y, z) &= \sum_{h_1} \sum_{h_2} \sum_{h_3} g(h_1, h_2, h_3) \exp \left[2\pi i \left(\frac{h_1 x}{a} + \frac{h_2 y}{b} + \frac{h_3 z}{c} \right) \right] \\ &= 0 \end{aligned} \right\} \begin{array}{l} \text{when } (x, y, z) \in V, \\ \text{when } (x, y, z) \notin V, \end{array} \quad (35)$$

where h_1, h_2, h_3 take on all possible integer values ($-\infty < h_j < \infty, j = 1, 2, 3$) and $g(h_1, h_2, h_3)$ are constants.

The Fourier transform, defined by (25), of the potential (35) is given by the expression

* See, for example a review article by M. Bertero and C. de Mol in *Progress in Optics*, Vol. XXXVI, ed. E. Wolf (Amsterdam, Elsevier, 1996), p. 129 *et seq.* Reconstruction of scattering potentials with special reference to extrapolation to the exterior of the Ewald limiting sphere has been discussed by T. Habashy and E. Wolf, *J. Mod. Opt.*, **41** (1994) 1679.

† See, for example B. A. Fuks, *Theory of Analytic Functions of Several Complex Variables* (Providence, RI, American Mathematical Society, 1963), p. 353 *et seq.*

‡ This theorem follows at once from a well-known result on analytic functions defined by definite integrals [see E. T. Copson, *An Introduction to the Theory of Functions of a Complex Variable* (London, Oxford University Press, 1955), Sec. 5.5].

$$\tilde{F}(K_x, K_y, K_z) = ABC\pi^3 \sum_{h_1} \sum_{h_2} \sum_{h_3} g(h_1, h_2, h_3) S(h_1, h_2, h_3; K_x, K_y, K_z), \quad (36)$$

with

$$S(h_1, h_2, h_3; K_x, K_y, K_z) = \operatorname{sinc} \left[\frac{1}{2} \left(\frac{2h_1}{a} - \frac{K_x}{\pi} \right) A \right] \operatorname{sinc} \left[\frac{1}{2} \left(\frac{2h_2}{b} - \frac{K_y}{\pi} \right) B \right] \operatorname{sinc} \left[\frac{1}{2} \left(\frac{2h_3}{c} - \frac{K_z}{\pi} \right) C \right], \quad (37)$$

where

$$\operatorname{sinc}(x) = \frac{\sin \pi x}{\pi x}. \quad (38)$$

The function $\operatorname{sinc}(x)$ is plotted in Fig. 13.5. We see that it decreases from the value unity at $x = 0$ to the value zero at $x = \pm 1/2$ and then oscillates with rapidly diminishing amplitude.

Suppose now that the linear dimensions of the scattering volume are large compared with the periods, i.e. that

$$A \gg a, \quad B \gg b, \quad C \gg c. \quad (39)$$

Under these circumstances the ratios A/a , B/b , C/c will each be large compared with unity and, consequently, in view of the behaviour of the function $\operatorname{sinc}(x)$, the expression S , defined by Eq. (37) and hence also the Fourier transform (36) of the scattering potential will have nonnegligible values only when

$$K_x \approx \frac{2\pi h_1}{a}, \quad K_y \approx \frac{2\pi h_2}{b}, \quad K_z \approx \frac{2\pi h_3}{c}. \quad (40)$$

Relation (27) (the analogue to the quantum mechanical momentum transfer equation) implies that the intensity of the scattered field in the far zone will be appreciable only in directions $\mathbf{s} \equiv (s_x, s_y, s_z)$ such that

$$s_x - s_{0x} = h_1 \frac{\lambda}{a}, \quad s_y - s_{0y} = h_2 \frac{\lambda}{b}, \quad s_z - s_{0z} = h_3 \frac{\lambda}{c}, \quad (41)$$

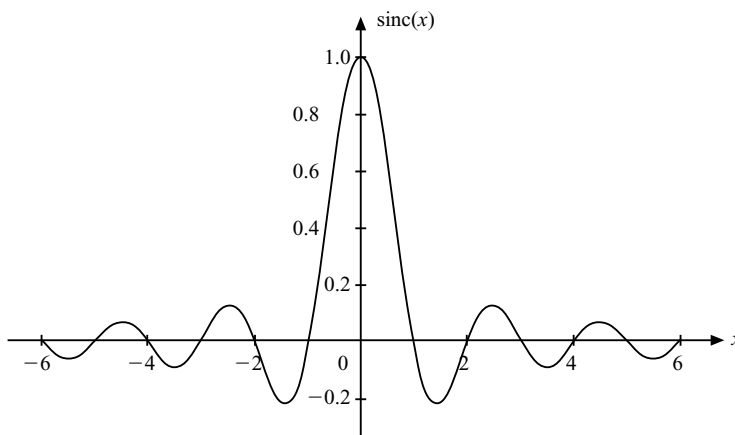


Fig. 13.5 The function $\operatorname{sinc}(x) = \sin(\pi x)/\pi x$.

where (s_{0x}, s_{0y}, s_{0z}) are the components of the unit vector \mathbf{s}_0 in the direction of propagation of the incident plane wave.

Formulae (41) are generalizations of the corresponding formulae [see §8.6 (8)] for one- and two-dimensional diffraction gratings (sometimes called line gratings and cross gratings respectively). However, there is an essential difference. Whilst for line gratings and cross gratings equations of the form (41) always have solutions for the directions \mathbf{s} of diffraction (there being one such equation for line gratings, two for cross gratings), this is not so for three-dimensional gratings (also called space gratings). Eq. (41) is a set of three equations for only two independent components of \mathbf{s} (say s_x and s_y), because the three components are related by the constraint $s_x^2 + s_y^2 + s_z^2 = 1$. Hence the three equations (41) can only be satisfied for some particular value of λ if the other parameters on the right-hand side are prescribed. This implies that whilst line gratings and cross gratings produce a continuous spectrum with incident light that contains a range of wavelengths, space gratings are selective: with every intensity maximum, labelled by a triplet of integers h_1, h_2, h_3 , there is associated a characteristic wavelength.

So far we have discussed the locations of the maxima of the intensities of the scattered field in the far zone. The actual values of the maxima, which are proportional to the squared modulus of the scattered field, are according to (23) and (26) proportional to $|\tilde{F}[k(\mathbf{s} - \mathbf{s}_0)]|^2$. Hence if the Fourier expansion coefficients $g(h_1, h_2, h_3)$ of the scattering potential are known the intensity maxima can be evaluated from (36), (27) and (41).

Because of the close analogy between scattering on a periodic potential and the diffraction of light by a grating one commonly speaks in such situations of diffraction rather than of scattering.

The results which we have just obtained have a close bearing on the technique of structure determination of solids from X-ray diffraction experiments. Most solids consist of a periodic arrangement of atoms in crystal lattices, the periodic element being called the *unit cell*. The separation between neighbouring atoms is typically of the order of an ångström unit (Å). This is the order of magnitude of the wavelengths of X-rays which are typically between about 0.1 Å and 10 Å. In 1912 Max von Laue predicted, before the atomic structure of matter and the wave nature of X-rays were generally accepted, that a solid would diffract a beam of X-rays in a similar way as a space grating would diffract light. This prediction was soon confirmed by experiment* and these early researches were the origin of a highly successful and important technique for studying the structure of matter.†

To indicate how the basic laws of the theory of X-ray diffraction follow from the theory of potential scattering we will restrict ourselves to the simplest case of so-called *orthorhombic crystals*. In such a crystal a unit cell is a rectangular parallelepiped. We

* W. Friedrich, P. Knipping and M. Laue, *Sber. bayer. Akad. Wiss.* (1912), 303 *et seq.* (theoretical part by M. Laue, experimental part by Friedrich and Knipping).

† For accounts of the development of this subject see P. P. Ewald, ed., *Fifty Years of X-ray Diffraction* (Utrecht, International Union of Crystallography, 1962) and G. E. Bacon, *X-ray and Neutron Diffraction* (Oxford, Pergamon Press, 1966). Bacon's book contains reprints of the classic papers on this subject. For more complete treatments of the theory of diffraction of X-rays see R. W. James, *Optical Principles of the Diffraction of X-rays*, Vol. 2 in *The Crystalline State*, eds W. H. Bragg and W. L. Bragg (London, G. Bell, 1948) or A. Guinier and D. L. Dexter, *X-rays Studies of Materials* (New York, Interscience Publishers, 1963).

take the x -, y -, z -axes along the direction of the edges of a unit cell and denote by a , b , c their lengths. Further we denote by A , B and C the lengths of the sides of the crystal and assume that $A \gg a$, $B \gg b$, $C \gg c$. Obviously the situation is completely analogous to that which we have encountered in considering scattering from a periodic potential. The only difference is that in the present case the wavelengths of the radiation (X-rays) are of the order of the lattice parameters a , b , c , whereas in the previous case (with light rather than X-rays) the wavelengths are generally much longer than the periodicities of the potential. Although we are restricting our discussion to diffraction by orthorhombic crystals, the so-called triclinic crystals can be treated in a similar manner, if an oblique instead of a rectangular coordinate system is used.

In the context of the theory of X-ray diffraction by crystals, (41) are known as the *von Laue equations* and are the basic equations of the theory. One may readily deduce from them another important law of the theory in the following way: Let us square both sides of each of the three equations (41), add them together and use the fact that $s_x^2 + s_y^2 + s_z^2 = 1$ and $s_{0x}^2 + s_{0y}^2 + s_{0z}^2 = 1$. One then obtains the equation

$$2 \sin(\theta/2) = \lambda/D, \quad (42)$$

where

$$D = \left[\left(\frac{h_1}{a} \right)^2 + \left(\frac{h_2}{b} \right)^2 + \left(\frac{h_3}{c} \right)^2 \right]^{-1/2} \quad (43)$$

and θ is the angle of scattering (diffraction), i.e. the angle between the direction of scattering (\mathbf{s}) and the direction of incidence (\mathbf{s}_0), so that

$$\mathbf{s} \cdot \mathbf{s}_0 = \cos \theta. \quad (44)$$

If the integers h_1 , h_2 , h_3 have a common factor which is an integer, n say, and if we set

$$h_1 = nh_1^*, \quad h_2 = nh_2^*, \quad h_3 = nh_3^* \quad (45)$$

and

$$D = \frac{d}{n}, \quad d = \left[\left(\frac{h_1^*}{a} \right)^2 + \left(\frac{h_2^*}{b} \right)^2 + \left(\frac{h_3^*}{c} \right)^2 \right]^{-1/2}, \quad (46)$$

(42) becomes

$$2d \sin \psi = n\lambda, \quad (47)$$

where

$$\psi = \theta/2. \quad (48)$$

Formula (47) is another basic result of the theory of X-ray diffraction by crystals, known as *Bragg's law*. It has a simple geometrical significance which we will now briefly discuss.

Let us consider a plane whose equation is

$$\frac{h_1^*}{a}x + \frac{h_2^*}{b}y + \frac{h_3^*}{c}z = n, \quad (49)$$

where n is an integer. Were the crystal unbounded such a plane, which we denote by π_n , would be called a *lattice plane*. It contains an infinite number of lattice points (corners of the unit cells). The numbers h_1^* , h_2^* and h_3^* are known as *Miller indices* of the lattice plane.

In the theory of X-ray diffraction by crystals, Bragg's law expresses the condition for constructive interference of rays reflected from successive lattice planes so as to produce intensity maxima. To demonstrate this fact let us consider a parallel beam of X-rays, incident in the direction \mathbf{s}_0 and reflected in direction \mathbf{s} . Let O_1 be a point on the lattice plane π_1 where an incident ray is reflected and let O_0 be the corresponding point on the lattice plane π_0 (see Fig. 13.6). The path difference Δ between the rays reflected at O_1 and O_0 is

$$\Delta = AO_1 + O_1B, \quad (50)$$

where A and B are the feet of the perpendiculars dropped from O_0 onto the rays incident and reflected at O_1 . The rays reflected at O_1 and O_0 will interfere constructively when

$$k\Delta = 2n\pi, \quad (51)$$

n being any integer. Let θ be, as before, the angle between the directions of the unit vectors \mathbf{s} and \mathbf{s}_0 and let ψ be the angle which an incident ray makes with a lattice plane. A simple geometrical argument shows that $\psi = \theta/2$ and consequently, as seen from (50) and from Fig. 13.6,

$$\Delta = 2d \sin \psi, \quad (52)$$

where d is the distance between the two neighbouring lattice planes π_0 and π_1 . Equating the two expressions (51) and (52) we see that the condition for constructive interference is

$$2d \sin \psi = n\lambda, \quad (53)$$

which is precisely Bragg's law (47).

One might well ask why the first Born approximation describes so well the intensity

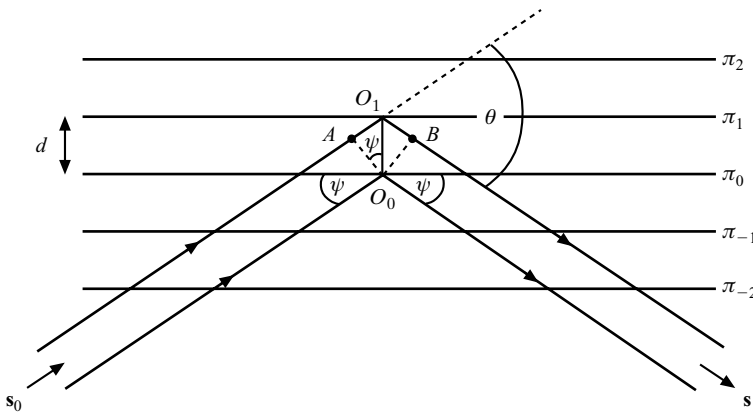


Fig. 13.6 Illustrating Bragg's law as a condition for constructive interference of rays reflected at lattice planes.

distribution produced by scattering of X-rays by crystals; for in this case the scattered field is strong in certain directions, contrary to the assumption of weak scattering, implicit in the use of that approximation. The explanation lies in the fact that, because of equal spacing between certain planes in a crystal (the lattice planes), interference between X-rays reflected from these planes, rather than scattering by the individual atoms, plays a major role in the formation of the observed field.

Max von Laue received the 1914 Nobel Prize for Physics for his discovery of the diffraction of X-rays by crystals. The 1915 Nobel Prize for Physics was awarded jointly to W. H. Bragg and to his son, W. L. Bragg, for their researches on the analysis of crystal structure by that technique.

Some of the concepts that we have encountered in our brief discussion of X-ray diffraction by crystals are of importance in holography, especially in connection with so-called volume holograms. Such holograms consist of three-dimensional sets of layers with periodic variation of the refractive index or of the absorption coefficients. Bragg's law plays a central role in the theory of such holograms. It is also of importance in acousto-optics.

13.1.4 Multiple scattering

Let us now return to the basic equation of potential scattering, taking the incident wave to be a plane wave [(16), with the frequency ω not displayed],

$$U(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V U(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r', \quad (54)$$

where

$$U^{(i)}(\mathbf{r}) = e^{ik_0 \mathbf{r}} \quad (55)$$

and

$$G(\mathbf{r}, \mathbf{r}') = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \quad (56)$$

As we noted earlier, if the scattering is weak ($|U^{(s)}| \ll |U^{(i)}|$), one might expect to obtain a good approximation to the total field if U is replaced by $U^{(i)}$ in the integrand on the right-hand side of (54). This gives the first-order Born approximation

$$U_1(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r'. \quad (57)$$

One might expect that an improved approximation is obtained if one substitutes U_1 for U in the integrand on the right-hand side of the integral equation (54). This leads to the so-called second-order Born approximation $U \approx U_2$,

$$U_2(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V U_1(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r'. \quad (58)$$

One can continue this procedure by next substituting U_2 for U in the integral in (54) etc. and one obtains the sequence of successive approximations

$$U_1(\mathbf{r}), U_2(\mathbf{r}), U_3(\mathbf{r}), \dots, U_n(\mathbf{r}), \dots, \quad (59)$$

where each term is obtained from the preceding one by means of the recurrence relation

$$U_{n+1}(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V U_n(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r'. \quad (60)$$

To gain some insight into the physical significance of the sequence (60), let us first re-write the expression (58) for U_2 in a more explicit form. If we substitute for U_1 from (57) and make a slight change in the notation we find that

$$U_2(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V d^3 r' F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') \left[U^{(i)}(\mathbf{r}') + \int_V U^{(i)}(\mathbf{r}'') F(\mathbf{r}'') G(\mathbf{r}' - \mathbf{r}'') d^3 r'' \right]$$

implying that

$$U_2(\mathbf{r}) = U^{(i)}(\mathbf{r}) + \int_V U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r' + \int_V \int_V U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r}' - \mathbf{r}'') F(\mathbf{r}'') G(\mathbf{r} - \mathbf{r}'') d^3 r' d^3 r''. \quad (61)$$

We see that the second term on the right is an integral over the scattering volume V and that the third term involves integration taken twice independently over that volume. If we continue this procedure we will evidently find that the expression U_n for the n th order approximation involves integrals taken once, twice, \dots , n times over the scattering volume. Because the formulae become more and more lengthy as n increases, one often expresses them in a symbolic form. In particular, equation (61) for U_2 may be written as

$$U_2 = U^{(i)} + U^{(i)} FG + U^{(i)} FGFG \quad (62)$$

and the expression for the general term, U_n , can be evidently written as

$$U_n = U^{(i)} + U^{(i)} FG + U^{(i)} FGFG + \dots + U^{(i)} \underbrace{FGFG \dots FG}_{n \text{ factors } FG}. \quad (63)$$

The physical significance of the successive terms is as follows: The product $U^{(i)}(\mathbf{r}') F(\mathbf{r}') d^3 r'$, in the integral in (57) and also the first integral on the right of (61) may be regarded as representing the response to the incident field of the volume region $d^3 r'$ around the point \mathbf{r}' of the scatterer. It acts as an effective source which makes a contribution $U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r} - \mathbf{r}') d^3 r'$ to the field at another point, \mathbf{r} , that may be situated either inside or outside V . Evidently the Green's function $G(\mathbf{r} - \mathbf{r}')$ acts as a *propagator* transferring the contribution from the point \mathbf{r}' to the point \mathbf{r} . The integral over the volume V thus represents the total contribution from all the volume elements of the scatterer. This process is known as *single scattering* and is illustrated in Fig. 13.7(a).

In addition to single scattering, there will also be contributions to the total field at \mathbf{r} which arise from other scattering processes. For example, the contribution $U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r}' - \mathbf{r}'') d^3 r'$ which reaches another point \mathbf{r}'' will itself be scattered, and consequently a volume element $d^3 r''$ around \mathbf{r}'' will give rise to another contribution, $U^{(i)}(\mathbf{r}') F(\mathbf{r}') G(\mathbf{r}' - \mathbf{r}'') d^3 r' F(\mathbf{r}'') G(\mathbf{r} - \mathbf{r}'') d^3 r''$ to the field at each point \mathbf{r} . The

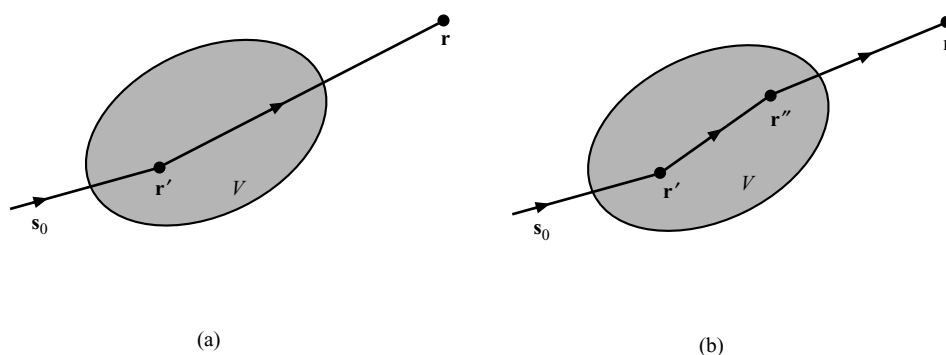


Fig. 13.7 Illustrating (a) single and (b) double scattering.

last term on the right of (60), representing the field at a point \mathbf{r} , arising from this process, expresses the effect of *double scattering*. It is illustrated in Fig. 13.7(b).

Evidently one can interpret all the successive terms in (63) in a similar way. Each successive term takes into account one more contribution of the elementary scattering process than does the previous one. The general term, $U^{(i)}FGFG \dots FG$ which contains n products FG is said to represent the effect of *multiple scattering* of order n .

Under suitable conditions, the sequence $U_1, U_2, \dots, U_n, \dots$, of successive approximations might be expected to converge to the exact solution of the integral equation of scattering, but conditions which ensure this are difficult to establish. The question of convergence is, however, of little practical consequence because it is seldom possible to carry out the calculations beyond the first- or the second-order approximation. The reason is clear if we note that each successive term in the sequence (63) involves integrations over domains of higher and higher dimensionality. In particular, as is seen from (57) and (61) the first-order Born approximation requires evaluation of a three-dimensional integral and the second-order one involves the evaluation of a six-dimensional integral.

Perturbation expansions of the type which we have briefly considered in this section have been investigated in the general theory of integral equations, where an expansion of the form (63) as $n \rightarrow \infty$ is known as the *Liouville–Neumann series*.

13.2 Principles of diffraction tomography for reconstruction of the scattering potential

In §4.11 we described the method of computerized tomography which makes it possible to determine the structure of three-dimensional objects (frequently their absorption coefficient) from measurements of the changes in the intensity of radiation which passes through the objects in different directions. The method is based on geometrical optics, which is adequate for the reconstruction when the wavelengths of the radiation that is employed (usually X-rays) are very short compared with the length scale of variation of the physical parameters of the object. However, X-rays are not suitable for probing certain soft tissues, because they penetrate them without any significant change. An important example where computerized tomography may not be reliable is in the detection of certain cancerous tumors in women's breasts. In such

cases ultrasonic waves rather than X-rays are often used. However, because the ultrasonic wavelengths, typically of the order of a millimetre (frequencies of the order of a megahertz) are comparable with the dimensions of the features of the object which one wishes to explore, relatively poor resolution is generally obtained. To achieve better resolution one must take diffraction into account. This can be done by using a different reconstruction procedure, known as *diffraction tomography*. Diffraction tomography with ultrasonic waves makes it possible to determine not only the distribution of the absorption coefficient throughout the object, but also the distribution of the real refractive index. However, diffraction tomography is computationally much more demanding than is computerized tomography and it is largely for this reason that it has not been so widely used.

We will confine our discussion of diffraction tomography mainly to the derivation of a central theorem relating to reconstruction by this technique.

13.2.1 Angular spectrum representation of the scattered field

The basic theorem concerning the reconstruction of three-dimensional objects is most easily derived from the so-called angular spectrum representation of the scattered field. We will therefore first discuss this representation, which we encountered in a more restrictive form in §11.4.2 in connection with certain two-dimensional problems.

We will base our analysis on the first-order Born approximation for the scattered field. It is given by the second term on the right-hand side of §3.1 (22), viz.,

$$U_1^{(s)}(\mathbf{r}) = \int_V F(\mathbf{r}') e^{ik s_0 \cdot \mathbf{r}'} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r'. \quad (1)$$

The spherical wave in the integrand in this integral may be represented in the following form, essentially due to H. Weyl:*

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = \frac{ik}{2\pi} \iint_{-\infty}^{\infty} \frac{1}{s_z} e^{ik[s_x(x-x') + s_y(y-y') + s_z(z-z')]} ds_x ds_y, \quad (2)$$

where $\mathbf{r} \equiv (x, y, z)$, $\mathbf{r}' \equiv (x', y', z')$ and

$$s_z = +\sqrt{1 - s_x^2 - s_y^2} \quad \text{when } s_x^2 + s_y^2 \leq 1, \quad (3a)$$

$$= +i\sqrt{s_x^2 + s_y^2 - 1} \quad \text{when } s_x^2 + s_y^2 > 1. \quad (3b)$$

Evidently s_x, s_y, s_z are components of a unit vector, but this vector is real only when $s_x^2 + s_y^2 \leq 1$. When $s_x^2 + s_y^2 > 1$ its z -component is imaginary.

Suppose now that the scatterer is situated within the region $0 \leq z \leq Z$ and let \mathcal{R}^- and \mathcal{R}^+ denote the half-spaces $z < 0$ and $z > Z$ on either side of the scatterer (see Fig. 13.8). If we substitute from (2) into (1) we obtain after some straightforward algebraic manipulation, including interchanging the order of integrations, the following expres-

* H. Weyl, *Ann. d. Physik*, **60** (1919), 481. This representation can be expressed in several different forms (see, for example, §11.7 (27)). For a derivation of the Weyl representation in the form given by (2) see L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge, Cambridge University Press, 1995), §3.2.4.

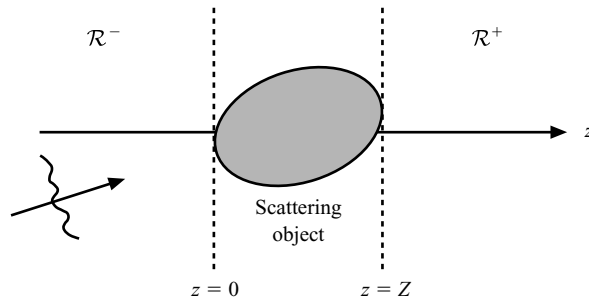


Fig. 13.8 Illustrating the notation relating to the angular spectrum representation of the scattered field.

sion for the scattered field $U_1^{(s)}(\mathbf{r})$ valid in the half-space \mathcal{R}^+ (upper sign) and \mathcal{R}^- (lower sign):

$$U_1^{(s)}(\mathbf{r}) = \iint_{-\infty}^{\infty} a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) e^{ik[s_x x + s_y y \pm s_z z]} ds_x ds_y. \quad (4)$$

Here

$$a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) = \frac{ik}{2\pi s_z} \int F(\mathbf{r}') e^{-ik[(s_x - s_{0x})x' + (s_y - s_{0y})y' + (\pm s_z - s_{0z})z']} d^3 r'. \quad (5)$$

Formula (4) is seen to represent the field $U_1^{(s)}(\mathbf{r})$ throughout the two half-spaces as a linear superposition of two kinds of plane waves: namely those for which s_z is given by (3a) and those for which it is given by (3b). The former are ordinary *homogeneous waves*, propagating away from the scatterer in direction $(s_x, s_y, \pm s_z)$; the latter are *evanescent waves*; their amplitude decays exponentially with increasing value of $|z|$. (See §11.4.2 and Fig. 13.9.)

Formula (4) is said to represent the scattered field in the half-spaces \mathcal{R}^+ and \mathcal{R}^- in the form of an *angular spectrum of plane waves*, which we already briefly encountered in §11.4. It is a *mode representation* of the field in the two half-spaces, because each of the plane waves satisfies the same equation as does the scattered field outside the scattering medium, namely the Helmholtz equation. Although the angular spectrum representation superficially resembles a Fourier integral representation, they must not be confused. In a Fourier integral all three variables s_x, s_y, s_z would have to be real; moreover, since $U_1^{(s)}(\mathbf{r})$ is a function of a three-dimensional vector \mathbf{r} , its Fourier representation would extend over the whole three-dimensional space, not over a two-dimensional (planar) domain, as is the case with the angular spectrum representation (4).*

We note that for homogeneous plane waves (with s_z real), (5) may be expressed in the form

* For fuller discussions of the angular spectrum representation see L. Mandel and E. Wolf, *loc. cit.* §3.2 and P. C. Clemmow, *The Plane Wave Spectrum Representation of Electromagnetic Fields* (Oxford, Pergamon Press, 1966).

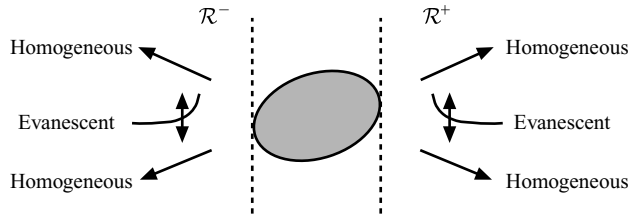


Fig. 13.9 Illustrating the types of plane wave modes which contribute to the scattered field in the half-spaces \mathcal{R}^+ and \mathcal{R}^- .

$$a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) = \frac{ik}{2\pi s_z} \tilde{F}[k(s_x - s_{0x}), k(s_y - s_{0y}), k(\pm s_z - s_{0z})], \quad (6)$$

where \tilde{F} is the Fourier transform defined by §13.1 (25), of the scattering potential. This formula shows that each homogeneous wave carries information about one and only one three-dimensional Fourier component of the scattering potential, namely the one which is labelled by the vector $\mathbf{K}^\pm = (K_x, K_y, K_z^{(\pm)})$, where

$$K_x = k(s_x - s_{0x}), \quad K_y = k(s_y - s_{0y}), \quad K_z^{(\pm)} = k(\pm s_z - s_{0z}). \quad (7)$$

However, the situation is quite different with evanescent waves, because for such waves s_{0z} is purely imaginary and hence $k(\pm s_z - s_{0z})$ is no longer the z -component of a real \mathbf{K} -vector which labels a Fourier component of the potential.

On comparing (6) with §13.1 (26) for the scattering amplitude $f_1(\mathbf{s}, \mathbf{s}_0)$ we see that the amplitude of each homogeneous plane wave in the angular spectrum representation of the scattered field is very simply related to the scattering amplitude, by the formula

$$a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) = \frac{ik}{2\pi} f_1(\mathbf{s}, \mathbf{s}_0), \quad (8)$$

where the upper sign is taken when $s_z > 0$ and the lower sign when $s_z < 0$.

13.2.2 The basic theorem of diffraction tomography

We note that if we eliminate the spectral amplitudes $a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y})$ of the homogeneous waves between (8) and (6) we will obtain the formula §13.1 (26), which makes it possible to determine the low spatial frequency components ($|\mathbf{K}| = k|\mathbf{s} - \mathbf{s}_0| \leq 2k$) of the scattering potential from far-zone measurements. However, in practice (especially with acoustical waves), the far zone is seldom accessible to measurements, and one can generally make measurements only closer to the scatterer. We will now show that the same information that can be deduced from far-zone data can also be obtained from measurements in two planes which are at arbitrary distances from the scatterer, one in the half-space \mathcal{R}^+ , the other in the half-space \mathcal{R}^- . This possibility is at the root of diffraction tomography.

Let $z = z^+$ be a plane in the half-space \mathcal{R}^+ and $z = z^-$ be a plane in the half-space \mathcal{R}^- (see Fig. 13.10). According to (4), the scattered field in the two planes is given by the integrals [writing now $U_1^{(s)}(x, y, z^{(\pm)}; \mathbf{s}_0)$ in place of $U_1^{(s)}(\mathbf{r})$]

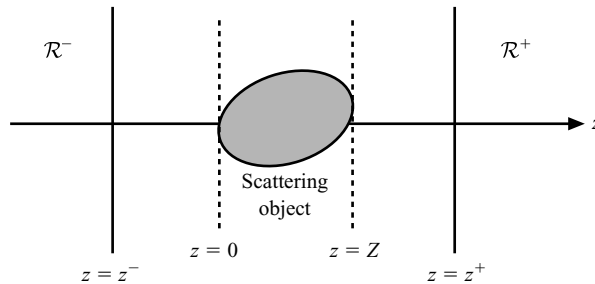


Fig. 13.10 Notation relating to the reconstruction of a scattering object from measurements of the scattered field across planes $z = z^-$ and $z = z^+$, one on each side of the scatterer.

$$U_1^{(s)}(x, y, z^{(\pm)}; \mathbf{s}_0) = \iint_{-\infty}^{\infty} a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) e^{ik(s_x x + s_y y \pm s_z z^{\pm})} ds_x ds_y. \quad (9)$$

Let us take the Fourier inverse of the scattered field $U_1^{(s)}$ in the two planes, with respect to the variables x and y . One then obtains the following expressions for the spectral amplitudes:

$$a^{(\pm)}(s_x, s_y; s_{0x}, s_{0y}) = \frac{1}{(2\pi)^2} k^2 \tilde{U}^{(s)}(ks_x, ks_y; z^{\pm}; \mathbf{s}_0) e^{\mp i k s_z z^{\pm}}, \quad (10)$$

where

$$\tilde{U}(f_x, f_y; z^{\pm}; \mathbf{s}_0) = \iint_{-\infty}^{\infty} U^{(s)}(x, y, z^{\pm}; \mathbf{s}_0) e^{-i(f_x x + f_y y)} dx dy. \quad (11)$$

We have obtained two expressions for the spectral amplitude. The first one, given by (6), applies only to the spectral amplitudes of the homogeneous waves and gives them in terms of the three-dimensional Fourier transform of the scattering potential. The other, (10), applies to both the homogeneous and the evanescent waves and expresses their spectral amplitudes in terms of the two-dimensional Fourier transform of the scattered field in the planes $z = z^+$ and $z = z^-$. Equating these two formulae, under the assumption that $s_x^2 + s_y^2 \leq 1$ (homogeneous waves) one obtains the relation

$$\tilde{F}[k(s_x - s_{0x}), k(s_y - s_{0y}), k(\pm s_z - s_{0z})] = \frac{ks_z}{2\pi i} \tilde{U}^{(s)}(ks_x, ks_y; z^{\pm}; \mathbf{s}_0) e^{\mp i k s_z z^{\pm}}. \quad (12)$$

If we set

$$f_x = ks_x, \quad f_y = ks_y, \quad f_z = ks_z = +(k^2 - f_x^2 - f_y^2)^{1/2} \quad (13)$$

and

$$K_x = f_x - ks_{0x}, \quad K_y = f_y - ks_{0y}, \quad K_z^{\pm} = \pm f_z - ks_{0z} \quad (14)$$

(12) may be expressed in the form

$$\tilde{F}(K_x, K_y, K_z^{\pm}) = \frac{f_z}{2\pi i} \tilde{U}^{(s)}(f_x, f_y; z^{\pm}; \mathbf{s}_0) e^{\mp i f_z z^{\pm}}. \quad (15)$$

In view of the inequality $s_x^2 + s_y^2 \leq 1$ appropriate to homogeneous waves, it follows from (13) that

$$f_x^2 + f_y^2 \leq k^2 \quad (16)$$

and, if we also use (14) we see that

$$|\mathbf{K}| \leq 2k. \quad (17)$$

Relation (15), together with (14), is the mathematical formulation of the basic theorem of diffraction tomography due to Wolf.* It shows how one can determine the low spatial-frequency components of the scattering potential, namely those for which the inequality (17) is satisfied, from measurements of the scattered fields in the two planes $z = z^+$ and $z = z^-$, one on each side of the scatterer, at arbitrary distances from it. It is to be noted that the Fourier components of the scattering potential which can be determined by this technique, constrained by the inequality (17), are precisely those whose representative \mathbf{K} -vectors have end points that are located inside the Ewald limiting sphere [see §13.1 (28)].

Several computational reconstruction techniques for diffraction tomography have been developed. One of them is the so-called filtered back-propagation algorithm, due to Devaney,† which may be regarded as a generalization of the back-projection algorithm of computerized tomography (see §4.11.5). Another reconstruction technique, utilizing frequency domain interpolation of the accessible Fourier components, was developed by Pan and Kak.‡

The theory of diffraction tomography was tested experimentally soon after it was formulated§ and has since then been applied in several fields, for example in optical microscopy to determine the variation of the refractive index throughout three-dimensional objects and in geophysics using acoustical and electromagnetic waves in prospecting for oil and gas.||

The basic formula (15) of diffraction tomography is valid only within the accuracy of the first-order Born approximation. In some cases, e.g. when the object is very small, certain computational difficulties are encountered even when scattering is weak.¶ When the object is large one may sometimes also encounter problems because the cumulative effect of small errors may become significant. In such situations it may be advantageous to use the so-called first Rytov approximation rather than the first Born approximation. We will briefly discuss the Rytov approximation in §13.5.

* E. Wolf, *Opt. Commun.*, **1**, (1969), 153.

† A. J. Devaney, *Ultrasonic Imaging*, **4** (1982), 336; *IEEE Trans. on Biomed. Eng.*, BME-**30** (1983), 377; also in *Inverse Methods in Electromagnetic Imaging*, Part 2, eds. W. M. Boerner *et al.*, (Hingham, MA, D. Reidel Public., 1985), p. 1107.

‡ S. X. Pan and A. C. Kak, *IEEE Trans. Acoust., Speech and Signal Processing*, AASP-**31** (1983), 1262. See also A. C. Kak and M. Slaney, *Principles of Computerized Tomographic Imaging* (New York, NY, The Institute of Electrical and Electronic Engineering, 1988), Sec. 6.4.1.

§ W. H. Carter, *J. Opt. Soc. Amer.*, **60** (1970), 306; W. H. Carter and P. C. Ho, *Appl. Opt.*, **13** (1974), 162; A. F. Fercher, H. Bartelt, H. Becker and E. Wiltshko, *Appl. Opt.*, **18** (1979), 2427.

|| For accounts of some of these investigations see, for example, J. J. Stamnes, L.-J. Gelius, I. Johansen and N. Sponheim in *Inverse Problems in Scattering and Imaging*, eds. M. Bertero and E. R. Pike (Bristol, Adam Hilger, 1992), p. 268; J. J. Stamnes and T. C. Wedberg in *Part. and Part. Syst. Charact.*, **12** (1995), 95; E. Wolf in *Trends in Optics*, ed. A. Consortini (San Diego, Academic Press, 1996), p. 83.

¶ See K. Iwata and R. Nagata, *Jap. J. Appl. Phys.*, **14** (1975), Suppl. 14-1, 379.

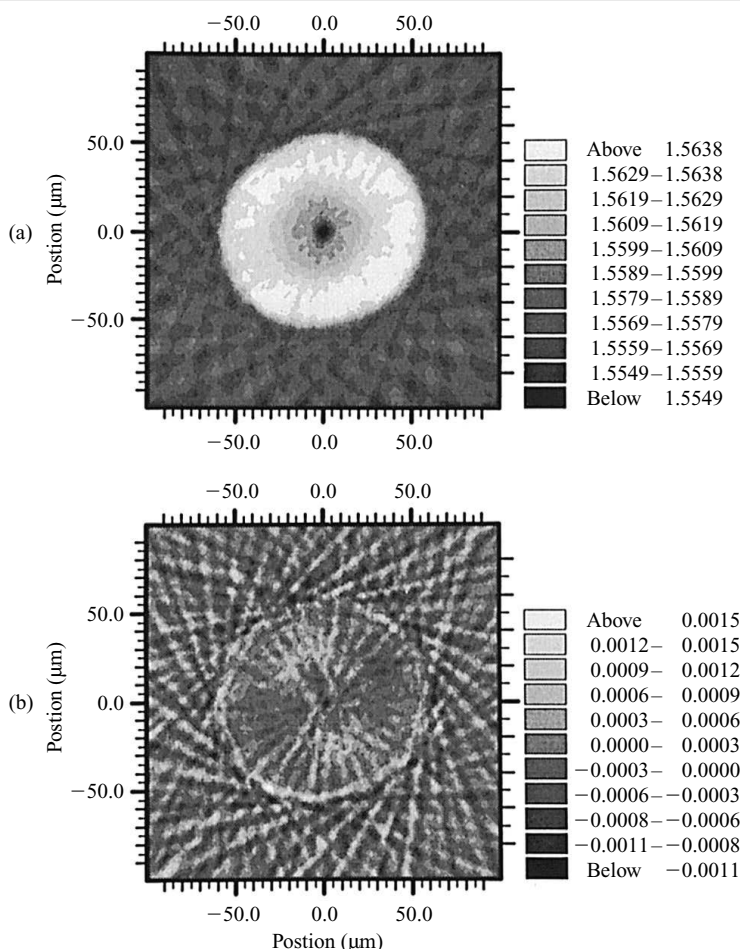


Fig. 13.11 The reconstructed real part (a) and imaginary part (b) of the complex refractive index distribution in a cross-section of a white horse hair. [After T. C. Wedberg and W. C. Wedberg, *J. Microscopy*, **177** (1995), 53.]

An example of the use of optical diffraction tomography is illustrated in Figs 13.11 and 13.12. The figures show the reconstructed refractive index distribution in a cross-section of a white horse hair.

13.3 The optical cross-section theorem

A quantity which is often of interest in the analysis of scattering experiments is not the scattered field itself but rather the rate at which energy is scattered and absorbed by the object. It turns out that there is a close relationship between the rate at which energy is lost from the incident field by these processes and the amplitude of the scattered field in the forward direction (the direction of incidence). This relationship is quantitatively expressed by the so-called *optical cross-section theorem* (often just called the optical theorem) which we will discuss in this section.

In electromagnetic theory the basic quantity associated with the propagation of

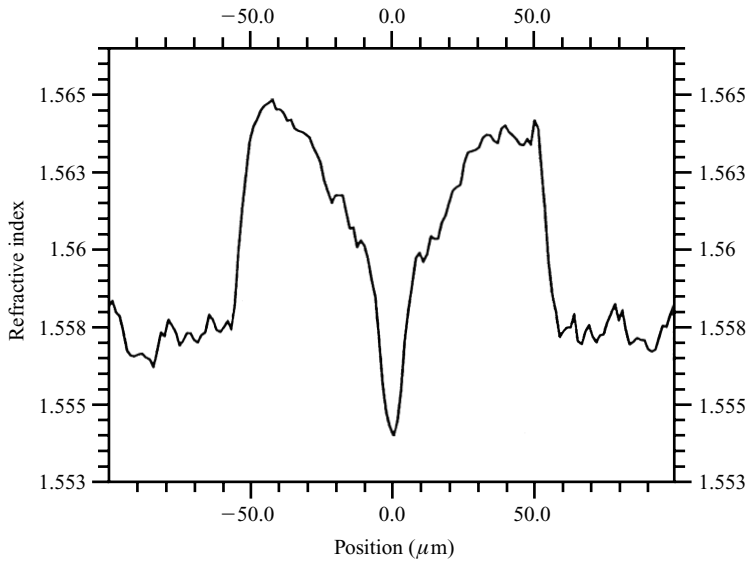


Fig. 13.12 Trace taken along the diameter of the reconstruction of the real part of the refractive index shown in Fig. 13.11(a). [After T. C. Wedberg and W. C. Wedberg, *J. Microscopy*, **177** (1995), 53.]

energy is the Poynting vector (§1.1.4). It is shown in Appendix XI [(10)] that the analogous quantity in scalar wave theory is the so-called *energy flux* vector. For a real monochromatic field

$$V^{(r)}(\mathbf{r}, t) = \mathcal{R}\{U(\mathbf{r})e^{-i\omega t}\}, \quad (1)$$

the average value of the energy flux vector, taken over an interval which is long compared to the period of the oscillations, is given by the expression

$$\langle \mathbf{F}(\mathbf{r}) \rangle = -i\beta[U^*(\mathbf{r})\nabla U(\mathbf{r}) - U(\mathbf{r})\nabla U^*(\mathbf{r})], \quad (2)$$

where β is a positive constant.

Suppose that a plane monochromatic wave of unit amplitude is incident on the scatterer in a direction specified by a real unit vector \mathbf{s}_0 . Its space-dependent part is then given by the expression

$$U^{(i)}(\mathbf{r}) = e^{ik\mathbf{s}_0 \cdot \mathbf{r}}. \quad (3)$$

As before we denote by $U^{(s)}(\mathbf{r})$ the scattered field and by $U(\mathbf{r})$ the total field so that

$$U(\mathbf{r}) = U^{(i)}(\mathbf{r}) + U^{(s)}(\mathbf{r}). \quad (4)$$

On substituting from (4) into (2) we obtain for the time-averaged energy flux vector the expression

$$\langle \mathbf{F}(\mathbf{r}) \rangle = \langle \mathbf{F}^{(i)}(\mathbf{r}) \rangle + \langle \mathbf{F}^{(s)}(\mathbf{r}) \rangle + \langle \mathbf{F}'(\mathbf{r}) \rangle, \quad (5)$$

where

$$\langle \mathbf{F}^{(i)}(\mathbf{r}) \rangle = -i\beta[U^{(i)*}(\mathbf{r})\nabla U^{(i)}(\mathbf{r}) - \text{cc}], \quad (6a)$$

$$\langle \mathbf{F}^{(s)}(\mathbf{r}) \rangle = -i\beta[U^{(s)*}(\mathbf{r})\nabla U^{(s)}(\mathbf{r}) - \text{cc}], \quad (6b)$$

$$\langle \mathbf{F}'(\mathbf{r}) \rangle = -i\beta[U^{(i)*}(\mathbf{r})\nabla U^{(s)}(\mathbf{r}) - U^{(s)}(\mathbf{r})\nabla U^{(i)*}(\mathbf{r}) - \text{cc}], \quad (6c)$$

and cc denotes the complex conjugate.

Let us now consider the outward flow of energy through a surface of a large sphere Σ of radius R , centred at some point O in the region occupied by the scatterer (see Fig. 13.13). It is given by the expression

$$\mathcal{W} = \iint_{\Sigma} \langle \mathbf{F}(\mathbf{r}) \rangle \cdot \mathbf{n} \, d\Sigma, \quad (7)$$

where \mathbf{n} is the unit outward normal to Σ . Were the scatterer a dielectric (i.e. a nonabsorbing medium) this integral would obviously have the value zero because energy would then be neither created nor destroyed by scattering. If, however the scatterer is a conducting body some of the energy is absorbed by it and the law of conservation of energy demands that the net outward energy flux through the surface Σ is equal in magnitude to the rate $\mathcal{W}^{(a)}$ at which absorption takes place. It then follows from (5) and (7) that

$$\mathcal{W} = -\mathcal{W}^{(a)} = \mathcal{W}^{(i)} + \mathcal{W}^{(s)} + \mathcal{W}', \quad (8)$$

where $\mathcal{W}^{(i)}$, $\mathcal{W}^{(s)}$ and \mathcal{W}' are the integrals of the radial components (i.e. components along the direction \mathbf{n} of the outward normal to Σ) $\langle \mathbf{F}^{(i)} \cdot \mathbf{n} \rangle$, $\langle \mathbf{F}^{(s)} \cdot \mathbf{n} \rangle$, $\langle \mathbf{F}' \cdot \mathbf{n} \rangle$ taken over the surface Σ of the sphere. Now since the incident field is assumed to satisfy the Helmholtz equation, $\mathcal{W}^{(i)} = 0$ as may be deduced from the differential form of the energy conservation law for monochromatic fields in free space [Appendix XI (13)] by

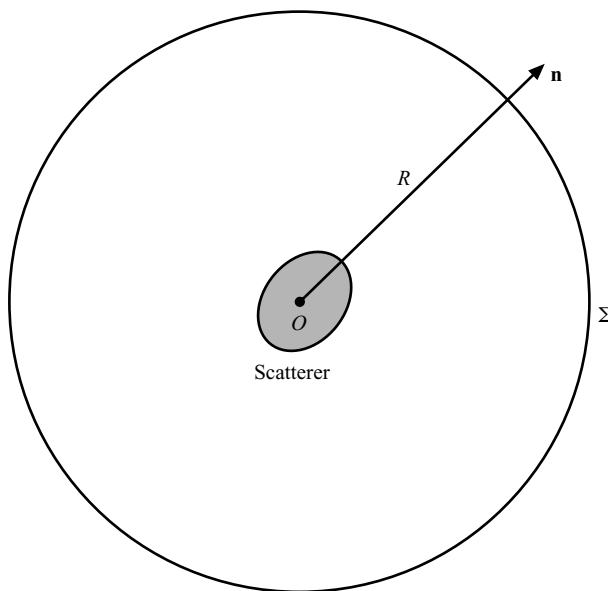


Fig. 13.13 Illustrating the notation relating to the formula (7).

application of Gauss' theorem. This result may also be verified more directly by a simple calculation. One has, on substituting from (3) into (6a),

$$\begin{aligned}\langle \mathbf{F}^{(i)}(\mathbf{r}) \rangle &= -i\beta[e^{-ik\mathbf{s}_0 \cdot \mathbf{r}} i k \mathbf{s}_0 e^{ik\mathbf{s}_0 \cdot \mathbf{r}} - \text{cc}] \\ &= 2\beta k \mathbf{s}_0.\end{aligned}\quad (9)$$

Hence

$$\mathcal{W}^{(i)} \equiv \iint_{\Sigma} \langle \mathbf{F}^{(i)}(\mathbf{r}) \rangle \cdot \mathbf{n} d\Sigma = 2\beta k \mathbf{s}_0 \cdot \iint_{\Sigma} \mathbf{n} d\Sigma. \quad (10)$$

It is clear by symmetry that the integral on the right of (10) has the value zero, as may be verified more explicitly by evaluating the integral on the right of (10) in spherical polar coordinates, with the polar axis along the \mathbf{s}_0 direction. Then $\mathbf{s}_0 \cdot \mathbf{n} = \cos \theta$, $d\Sigma = R^2 \sin \theta d\theta d\phi$, ($0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$), and it follows that

$$\mathcal{W}^{(i)} = 0, \quad (11)$$

as expected.

On making use of this result in (8) and recalling that \mathcal{W}' is the integral over Σ of the normal component of the expression (6c) it follows that

$$\begin{aligned}\mathcal{W}^{(s)} + \mathcal{W}^{(a)} &= -\mathcal{W}' \\ &= i\beta \iint_{\Sigma} [U^{(i)\star}(\mathbf{r}) \nabla U^{(s)}(\mathbf{r}) - U^{(s)}(\mathbf{r}) \nabla U^{(i)\star}(\mathbf{r}) - \text{cc}] \cdot \mathbf{n} d\Sigma.\end{aligned}\quad (12)$$

Since the incident field is the plane wave given by (3) and the scattered field in the far zone is given by §13.1 (20), viz.

$$U^{(s)}(r\mathbf{s}) = f(\mathbf{s}, \mathbf{s}_0) \frac{e^{ikr}}{r}, \quad (13)$$

where $f(\mathbf{s}, \mathbf{s}_0)$ is the scattering amplitude at frequency ω , one readily finds that on the large spherical surface Σ of radius R (see Fig. 13.13)

$$U^{(i)\star} \nabla U^{(s)} - U^{(s)} \nabla U^{(i)\star} = \frac{ik}{R} (\mathbf{s} + \mathbf{s}_0) f(\mathbf{s}, \mathbf{s}_0) e^{-ikR\mathbf{s} \cdot (\mathbf{s}_0 - \mathbf{s})}. \quad (14)$$

Next we substitute from (14) into (12). To evaluate the resulting integral we make use of a mathematical lemma due to D. S. Jones (see Appendix XII) which asserts that when R is large and G is an arbitrary function of \mathbf{n} ,

$$\frac{1}{R} \iint_{\Sigma} G(\mathbf{n}) e^{-ik(\mathbf{s}_0 \cdot \mathbf{n})R} d\Sigma \sim \frac{2\pi i}{k} [G(\mathbf{s}_0) e^{-ikR} - G(-\mathbf{s}_0) e^{ikR}]. \quad (15)$$

Hence, using (14) and this lemma it follows that

$$\iint_{\Sigma} (U^{(i)\star} \nabla U^{(s)} - U^{(s)} \nabla U^{(i)\star}) \cdot \mathbf{n} d\Sigma \sim -4\pi f(\mathbf{s}_0, \mathbf{s}_0) \quad (16)$$

and, consequently, we obtain from (12) the following expression for the sum $\mathcal{W}^{(s)} + \mathcal{W}^{(a)}$:

$$\begin{aligned}\mathcal{W}^{(s)} + \mathcal{W}^{(a)} &= -4\pi i \beta [f(\mathbf{s}_0, \mathbf{s}_0) - f^*(\mathbf{s}_0, \mathbf{s}_0)] \\ &= 8\pi \beta \mathcal{I} f(\mathbf{s}_0, \mathbf{s}_0),\end{aligned}\quad (17)$$

where \mathcal{I} denotes the imaginary part.

Relation (17) implies that *the rate at which the energy is removed from the incident plane wave by the processes of scattering and absorption is proportional to the imaginary part of the scattering amplitude for scattering in the forward direction $\mathbf{s} = \mathbf{s}_0$, i.e. to $f(\mathbf{s}_0, \mathbf{s}_0)$, usually called the forward scattering amplitude.*

The ratio Q between the rate of dissipation of energy ($\mathcal{W}^{(s)} + \mathcal{W}^{(a)}$) and the rate $|\langle \mathbf{F}^{(i)} \rangle|$ at which energy is incident on a unit cross-sectional area of the scatterer perpendicular to the direction \mathbf{s}_0 of propagation of the incident wave is called the *extinction cross-section* of the scattering object. From (17) and (9) it follows that

$$Q = Q^{(s)} + Q^{(a)} = \frac{\mathcal{W}^{(s)} + \mathcal{W}^{(a)}}{|\langle \mathbf{F}^{(i)} \rangle|} = \frac{4\pi}{k} \mathcal{I} f(\mathbf{s}_0, \mathbf{s}_0). \quad (18)$$

This formula is the mathematical formulation of the optical cross-section theorem (usually called the optical theorem). In the domain of classical optics it appears to have been first derived by van de Hulst.*

One may define the *scattering cross-section* $Q^{(s)}$ and the *absorption cross-section* $Q^{(a)}$ of the obstacle in a similar way,

$$Q^{(s)} = \frac{\mathcal{W}^{(s)}}{|\langle \mathbf{F}^{(i)} \rangle|}, \quad Q^{(a)} = \frac{\mathcal{W}^{(a)}}{|\langle \mathbf{F}^{(i)} \rangle|}, \quad (19)$$

and evidently $Q = Q^{(s)} + Q^{(a)}$. For a nonabsorbing obstacle $Q^{(a)} = 0$ and the extinction cross-section is then equal to the scattering cross-section.

The scattering cross-section $Q^{(s)}$ may be expressed in a simple form in terms of the scattering amplitude $f(\mathbf{s}, \mathbf{s}_0)$. To show this let us first consider the flux vector $\mathbf{F}^{(s)}$ of the scattered field in the far zone. On substituting from (13) into (6b), remembering that the field point is now in the far zone at distance R in the direction of a unit vector \mathbf{s} , we have

$$\langle \mathbf{F}^{(s)}(R\mathbf{s}) \rangle \sim \frac{2\beta k}{R^2} |f(\mathbf{s}, \mathbf{s}_0)|^2 \mathbf{s}, \quad \text{as } R \rightarrow \infty \text{ with } \mathbf{s} \text{ fixed.} \quad (20)$$

The rate at which energy crosses the large sphere Σ in the far zone is (noting that $\mathbf{s} = \mathbf{n}$ now),

$$\mathcal{W}^{(s)} = \iint_{\Sigma} \langle \mathbf{F}^{(s)}(r\mathbf{s}) \rangle \cdot \mathbf{s} \, d\Sigma = 2\beta k \int_{4\pi} |f(\mathbf{s}, \mathbf{s}_0)|^2 \, d\Omega, \quad (21)$$

where $d\Omega = d\Sigma/R^2$ is the element of solid angle subtended at the origin O by the element $d\Sigma$ and the integration extends over the whole 4π solid angle generated by the

* H. C. van de Hulst, *Physica*, **15** (1949), 740. There is an analogous theorem for atomic collisions [see E. Feenberg, *Phys. Rev.*, **40** (1932), 40; M. Lax, *Phys. Rev.*, (2), **78** (1950), 306]. An account of the history of the theorem was given by R. G. Newton, *Amer. J. Phys.*, **44** (1976), 639.

\mathbf{s} directions. Recalling that according to (9) $\langle \mathbf{F}^{(i)} \rangle = 2\beta k \mathbf{s}_0$, it follows that the scattering cross-section is given by the simple expression

$$Q^{(s)} \equiv \frac{\mathcal{W}^{(s)}}{|\langle \mathbf{F}^{(i)} \rangle|} = \int_{4\pi} |f(\mathbf{s}, \mathbf{s}_0)|^2 d\Omega. \quad (22)$$

For obvious reasons the quantity $|f(\mathbf{s}, \mathbf{s}_0)|^2$, which is often denoted as $dQ^{(s)}/d\Omega$, is called the *differential scattering cross-section*.

Let us consider the value of the extinction cross-section Q for an obstacle that does not transmit an appreciable fraction of the incident light. We also assume that the linear dimensions of the obstacle are large compared to the wavelength. In this case the Huygens–Kirchhoff theory applies and the main contribution to the forward scattering arises from Fraunhofer diffraction. Let \mathcal{A} be the ‘shadow region’ and \mathcal{A}' the unobstructed portion of a linearly polarized plane wave incident upon the obstacle (Fig. 13.14) and consider the scattered field $U^{(s)}$ at a point $P(\mathbf{r})$ at a large distance from the obstacle. If the angles of incidence and scattering are small we have according to the Huygens–Fresnel principle and Babinet’s principle [§8.3 (21)]

$$U^{(s)}(\mathbf{r}) = \frac{i}{\lambda} \iint_{\mathcal{A}} \frac{e^{ikr}}{r} dS, \quad (23)$$

where $\lambda = 2\pi/k$ is the wavelength associated with the wave number k , if the angle of diffraction is small. Since P is very far away from the obstacle in the direction of propagation of the incident wave (forward direction), r may be taken to be a constant and (23) gives

$$U^{(s)}(r\mathbf{s}_0) = \frac{i}{\lambda} D \frac{e^{ikr}}{r}, \quad (24)$$

where D is the geometrical cross-section of the obstacle (the area \mathcal{A}). Hence in this case the forward scattering amplitude $f(\mathbf{s}_0, \mathbf{s}_0)$ is equal to iD/λ and (18) shows that

$$Q = 2D. \quad (25)$$

Thus the extinction cross-section of a large opaque obstacle is equal to twice its

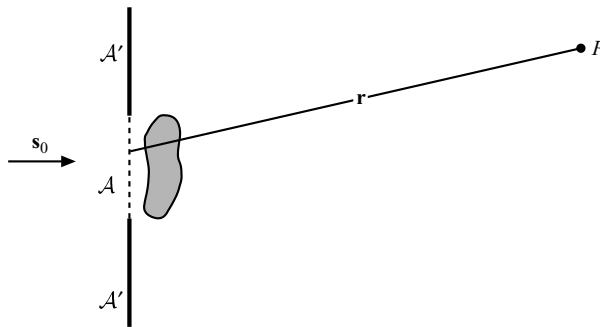


Fig. 13.14 Illustrating the notation used in (23) and (24), relating to the extinction cross-section of a large opaque obstacle. The region \mathcal{A} has geometrical cross-section D .

geometrical cross-section. This result appears somewhat paradoxical at first sight, as one might have expected that with a large obstacle the geometrical optics approximation would apply, and in this approximation the extinction cross-section is equal to D . The explanation of this apparent contradiction* is that no matter how large the obstacle may be and no matter how far away from it the field is considered, there is always a narrow region – the neighbourhood of the edge of the geometrical shadow – where the geometrical optics approximation does not hold. In addition to the light intercepted by the obstacle (lost by reflection and absorption), with cross-section D , there is an additional contribution to the extinction, arising from the neighbourhood of the edge of the shadow and this contribution is evidently also equal to D . In order to verify the relation (25) by experiment one must collect the light over a sufficiently wide area and far enough away from the obstacle.†

There is an interesting generalization of the optical cross-section theorem (18) which we will now briefly discuss.

Let us now consider two monochromatic fields of the same frequency ω (time-dependent factor $\exp(-i\omega t)$ and the argument ω in various expressions being understood), $U_1^{(i)}(\mathbf{r})$ and $U_2^{(i)}(\mathbf{r})$, incident on a scattering object and let $U_1(\mathbf{r})$ and $U_2(\mathbf{r})$ be the total fields which they generate. These fields satisfy the basic equation §13.1 (5) of scattering, viz.

$$\nabla^2 U_j(\mathbf{r}) + k^2 U_j(\mathbf{r}) = -4\pi F(\mathbf{r}) U_j(\mathbf{r}), \quad (j = 1, 2), \quad (26)$$

where $F(\mathbf{r})$ represents the scattering potential. It follows from (26) that

$$U_2^* \nabla^2 U_1 - U_1 \nabla^2 U_2^* = -8\pi i U_1 U_2^* \mathcal{I}F. \quad (27)$$

Let us integrate the normal components of the expression (27) over the large sphere Σ and let us apply Green's theorem to the integral on the left. This gives the formula

$$\iint_{\Sigma} (U_2^* \nabla U_1 - U_1 \nabla U_2^*) \cdot \mathbf{n} \, d\Sigma = 2i\mathcal{W}_{12}, \quad (28)$$

where

$$\mathcal{W}_{12} = -4\pi \int_D U_1(\mathbf{r}) U_2^*(\mathbf{r}) \mathcal{I}F(\mathbf{r}) d^3r. \quad (29)$$

Suppose that the incident fields $U_1^{(i)}$ and $U_2^{(i)}$ are plane waves which propagate in directions specified by real unit vectors \mathbf{s}_1 and \mathbf{s}_2 respectively. Then, according to §13.1 (19), the total fields in the far zone of the scatterer are given by the expressions

$$U_j(R\mathbf{s}) \sim e^{ikR\mathbf{s}\cdot\mathbf{s}_j} + f(\mathbf{s}, \mathbf{s}_j) \frac{e^{ikR}}{R}, \quad (j = 1, 2). \quad (30)$$

* There is an analogous paradox in the quantum theory of collisions, first noted by H. S. W. Massey and C. B. O. Mohr, *Proc. Roy. Soc. A*, **141** (1933), 434.

† It follows from a careful analysis leading to lemma (15), that the portion of Σ which contributes appreciably to Q subtends at the centre of S a solid angle of order $(kR)^{-\beta}$, where $1 > \beta > 4/5$ [see D. S. Jones, *Proc. Camb. Phil. Soc.*, **48** (1952), 733]. For a fuller discussion of the extinction cross-section of a large obstacle and the role played by the geometrical shadow see D. Sinclair, *J. Opt. Soc. Amer.*, **37** (1947), 475 and L. Brillouin, *J. Appl. Phys.*, **20** (1949), 1110.

Using (30) one finds after a long but straightforward calculation that on the sphere Σ ,

$$\begin{aligned} (U_2^* \nabla U_1 - U_1 \nabla U_2^*) \cdot \mathbf{n} &= ik \mathbf{s} \cdot (\mathbf{s}_1 + \mathbf{s}_2) e^{ikR\mathbf{s} \cdot (\mathbf{s}_1 - \mathbf{s}_2)} \\ &\quad + ik(1 + \mathbf{s} \cdot \mathbf{s}_2) f(\mathbf{s}, \mathbf{s}_1) \frac{e^{ikR(1 - \mathbf{s} \cdot \mathbf{s}_2)}}{R} \\ &\quad + ik(1 + \mathbf{s} \cdot \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2) \frac{e^{-ikR(1 - \mathbf{s} \cdot \mathbf{s}_1)}}{R} \\ &\quad + \frac{2ik}{R^2} f^*(\mathbf{s}, \mathbf{s}_2) f(\mathbf{s}, \mathbf{s}_1), \end{aligned} \quad (31)$$

where we have used the fact that $\mathbf{n} = \mathbf{s}$ on Σ .

On substituting from (31) into the integral on the left of (28) it is clear that one has to evaluate four integrals. Let us consider them separately.

The first integral is readily seen to have zero value, i.e.

$$ik \iint_{\Sigma} \mathbf{s} \cdot (\mathbf{s}_1 + \mathbf{s}_2) e^{ikR\mathbf{s} \cdot (\mathbf{s}_1 - \mathbf{s}_2)} d\Sigma = 0. \quad (32)$$

This can be verified most simply by considering the situation when $F \equiv 0$, i.e. when the scatterer is absent. In this case the quantity \mathcal{W}_{12} , defined by (29) has zero value and $U_j = U_j^{(i)} = \exp(ik\mathbf{s}_j \cdot \mathbf{r})$ ($j = 1, 2$). With these expressions for U_j , (32) follows at once from (28).

The second integral and the third integral can be evaluated by the use of Jones' lemma, expressed by (15), and one finds, recalling that $\mathbf{R} = R\mathbf{s}$,

$$ik \iint_{\Sigma} (1 + \mathbf{s} \cdot \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2) \frac{e^{-ik(R - \mathbf{s}_1 \cdot \mathbf{R})}}{R} d\Sigma = 4\pi f^*(\mathbf{s}_1, \mathbf{s}_2) \quad (33)$$

and that

$$ik \iint_{\Sigma} (1 + \mathbf{s} \cdot \mathbf{s}_2) f(\mathbf{s}, \mathbf{s}_1) \frac{e^{ik(R - \mathbf{s}_2 \cdot \mathbf{R})}}{R} d\Sigma = -4\pi f(\mathbf{s}_2, \mathbf{s}_1). \quad (34)$$

The fourth integral over the large sphere Σ can be re-written in the form

$$2ik \iint_{\Sigma} \frac{f(\mathbf{s}, \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2)}{R^2} d\Sigma = 2ik \iint_{4\pi} f(\mathbf{s}, \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2) d\Omega, \quad (35)$$

where the integrations extend over the whole 4π solid angle of directions generated by the unit vector \mathbf{s} .

On substituting the long expression (31) into (28) and using the values of the four integrals (32)–(35) we obtain the important result that

$$2\pi[f(\mathbf{s}_2, \mathbf{s}_1) - f^*(\mathbf{s}_1, \mathbf{s}_2)] = ik \iint_{4\pi} f(\mathbf{s}, \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2) d\Omega - i\mathcal{W}_{12}. \quad (36)$$

This formula is known as the *generalized optical theorem*, because with the choice $\mathbf{s}_2 = \mathbf{s}_1 = \mathbf{s}_0$ it reduces to the optical cross-section theorem (17), as we will now show.

It follows from (36) on setting $\mathbf{s}_2 = \mathbf{s}_1 = \mathbf{s}_0$ that

$$4\pi \mathcal{I}f(\mathbf{s}_0, \mathbf{s}_0) = k \iint_{4\pi} |f(\mathbf{s}, \mathbf{s}_0)|^2 d\Omega - \mathcal{W}_{00}. \quad (37)$$

Now according to (22) the integral on the right is equal to the scattering cross-section $Q^{(s)}$. Hence (37) implies that

$$Q^{(s)} = \frac{4\pi}{k} \mathcal{I}f(\mathbf{s}_0, \mathbf{s}_0) + \frac{1}{k} \mathcal{W}_{00}. \quad (38)$$

Further, it follows from (28) (since $\mathbf{n} = \mathbf{s}$ on Σ) that

$$\frac{1}{k} \mathcal{W}_{00} = \frac{1}{2ik} \iint_{\Sigma} (U_0^* \nabla U_0 - U_0 \nabla U_0^*) \cdot \mathbf{s} d\Sigma \quad (39)$$

or, using (2) and (9),

$$\frac{1}{k} \mathcal{W}_{00} = \frac{1}{|\langle \mathbf{F}^{(i)}(\mathbf{r}) \rangle|} \iint_{\Sigma} \langle \mathbf{F}(\mathbf{r}) \rangle \cdot \mathbf{s} d\Sigma. \quad (40)$$

The integral on the right represents the average rate at which energy crosses the large sphere Σ in the outward direction; it must be equal in magnitude but opposite in sign to the rate at which energy is absorbed by the scattering medium. Hence

$$\frac{1}{k} \mathcal{W}_{00} = -Q^{(a)}, \quad (41)$$

where $Q^{(a)}$ is the absorption cross-section of the scatterer. If we substitute from (41) into (38) and recall that $Q^{(s)} + Q^{(a)}$ is the extinction cross-section Q , (38) reduces to the optical cross-section theorem expressed by (18). Hence (36) is, indeed, a generalization of the optical cross-section theorem.

We note that when the scatterer is nonabsorbing, the imaginary part of the scattering potential [defined by §13.1 (6)] is zero and so is, therefore, the term \mathcal{W}_{12} defined by (28). The generalized optical theorem (36) then reduces to

$$2\pi[f(\mathbf{s}_2, \mathbf{s}_1) - f^*(\mathbf{s}_1, \mathbf{s}_2)] = ik \iint_{4\pi} f(\mathbf{s}, \mathbf{s}_1) f^*(\mathbf{s}, \mathbf{s}_2) d\Omega. \quad (42)$$

In the quantum theory of potential scattering this formula is often called the *unitary relation*.*

13.4 A reciprocity relation

Another general result of the scattering theory is a certain reciprocity theorem. It can be derived by a somewhat similar mathematical argument as we used in the preceding section in connection with the optical cross-section theorem.

Let us again consider two fields $U_1^{(i)}(\mathbf{r})$ and $U_2^{(i)}(\mathbf{r})$ incident on a scatterer and let

* See, for example, A. G. Sitenko, *Scattering Theory* (Berlin, Springer, 1975), Sec. 5.2.

$U_1(\mathbf{r})$ and $U_2(\mathbf{r})$ be the total fields (incident + scattered). Eq. §13.3 (26) then applies and, consequently,

$$U_2 \nabla^2 U_1 - U_1 \nabla^2 U_2 = 0. \quad (1)$$

On integrating this equation throughout the interior of the large sphere Σ and using Green's theorem it follows that

$$\iint_{\Sigma} (U_2 \nabla U_1 - U_1 \nabla U_2) \cdot \mathbf{n} \, d\Sigma = 0, \quad (2)$$

where \mathbf{n} denotes the unit outward normal to Σ .

Let us assume that the incident fields are plane waves of unit amplitudes, propagating in directions specified by real unit vectors \mathbf{s}_1 and \mathbf{s}_2 , i.e.

$$U_j^{(i)}(\mathbf{r}) = e^{ik\mathbf{s}_j \cdot \mathbf{r}}, \quad (j = 1, 2). \quad (3)$$

The total fields are then given by the expressions §13.3 (30). Using these expressions we readily find that on Σ

$$\begin{aligned} (U_2 \nabla U_1 - U_1 \nabla U_2) \cdot \mathbf{n} &= ik\mathbf{s} \cdot (\mathbf{s}_1 - \mathbf{s}_2) e^{ikR\mathbf{s} \cdot (\mathbf{s}_1 + \mathbf{s}_2)} \\ &\quad - ik(1 - \mathbf{s} \cdot \mathbf{s}_1) f(\mathbf{s}, \mathbf{s}_2) \frac{e^{ikR(1 + \mathbf{s}_1 \cdot \mathbf{s})}}{R} \\ &\quad + ik(1 - \mathbf{s} \cdot \mathbf{s}_2) f(\mathbf{s}, \mathbf{s}_1) \frac{e^{ik(1 + \mathbf{s}_2 \cdot \mathbf{s})}}{R}, \end{aligned} \quad (4)$$

where we have used the fact that $\mathbf{n} = \mathbf{s}$ and $\mathbf{R} = R\mathbf{s}$ on Σ .

Next we substitute from (4) into (2). Evidently we must evaluate three integrals. The first integral is identical with the integral which appears on the left-hand side of §13.3 (32), with \mathbf{s}_2 replaced by $-\mathbf{s}_2$. Making this change in §13.3 (32) it follows that

$$ik \iint_{\Sigma} \mathbf{s} \cdot (\mathbf{s}_1 - \mathbf{s}_2) e^{ikR\mathbf{s} \cdot (\mathbf{s}_1 + \mathbf{s}_2)} \, d\Sigma = 0. \quad (5)$$

The other two integrals may be evaluated by the use of Jones' lemma [§13.3 (15)] and one finds that

$$ik \iint_{\Sigma} (1 - \mathbf{s} \cdot \mathbf{s}_1) f(\mathbf{s}, \mathbf{s}_2) \frac{e^{ikR(1 + \mathbf{s}_1 \cdot \mathbf{s})}}{R} \, d\Sigma = -4\pi f(-\mathbf{s}_1, \mathbf{s}_2) \quad (6)$$

and

$$ik \iint_{\Sigma} (1 - \mathbf{s} \cdot \mathbf{s}_2) f(\mathbf{s}, \mathbf{s}_1) \frac{e^{ikR(1 + \mathbf{s}_2 \cdot \mathbf{s})}}{R} \, d\Sigma = -4\pi f(-\mathbf{s}_2, \mathbf{s}_1). \quad (7)$$

On integrating (4) over the sphere Σ , making use of (5)–(7) and substituting the resulting expression into (2) we find that $f(-\mathbf{s}_1, \mathbf{s}_2) = f(-\mathbf{s}_2, \mathbf{s}_1)$. If we replace \mathbf{s}_2 by $-\mathbf{s}_2$ we obtain the following *reciprocity relation*:*

* An analogous reciprocity relation for the electromagnetic field has been derived by A. T. de Hoop, *Appl. Sci. Res. B* (1959–1960), 135.

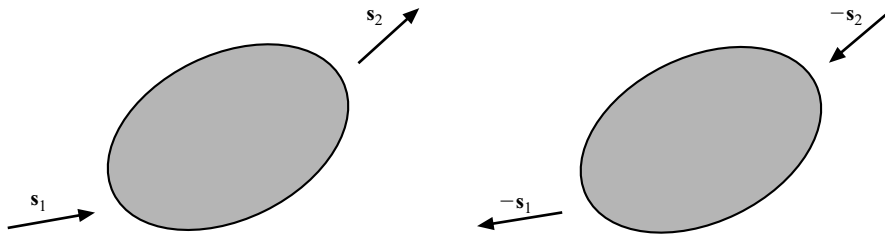


Fig. 13.15 Illustrating the reciprocity theorem expressed by (8).

$$f(\mathbf{s}_2, \mathbf{s}_1) = f(-\mathbf{s}_1, -\mathbf{s}_2). \quad (8)$$

This relation shows that *the scattering amplitude in direction \mathbf{s}_2 , when a monochromatic plane wave of unit amplitude is incident on the scatterer in direction \mathbf{s}_1 , is equal to the scattering amplitude in direction $-\mathbf{s}_1$ when a monochromatic plane wave of unit amplitude is incident on the scatterer in direction $-\mathbf{s}_2$* . This result is illustrated in Fig. 13.15.

13.5 The Rytov series

Instead of representing the solution of the basic integral equation §13.1(16) of scattering as a perturbation series which we briefly discussed in §13.1.4, one sometimes uses a different expansion due to Rytov.* The Rytov expansion is frequently used in problems of wave propagation in random media and in diffraction tomography. In this section we will give a brief account of this alternative technique.

We again begin with §13.1 (5), viz.

$$\nabla^2 U(\mathbf{r}, \omega) + k^2 U(\mathbf{r}, \omega) = -4\pi F(\mathbf{r}, \omega) U(\mathbf{r}, \omega), \quad (1)$$

where

$$F(\mathbf{r}, \omega) = \frac{1}{4\pi} k^2 [n^2(\mathbf{r}, \omega) - 1] \quad (2)$$

is the scattering potential, $n(\mathbf{r})$ being the refractive index. The essence of the Rytov procedure is to express $U(\mathbf{r}, \omega)$ in the form

$$U(\mathbf{r}, \omega) = e^{\psi(\mathbf{r}, \omega)}, \quad (3)$$

where ψ is generally complex, and to expand ψ rather than U in a perturbation series.

Let $A(\mathbf{r}, \omega)$ and $\phi(\mathbf{r}, \omega)$ be the amplitude and the (real) phase of $U(\mathbf{r}, \omega)$, i.e.,

$$U(\mathbf{r}, \omega) = A(\mathbf{r}, \omega) e^{i\phi(\mathbf{r}, \omega)}. \quad (4)$$

Then evidently

$$\psi(\mathbf{r}, \omega) = \ln A(\mathbf{r}, \omega) + i\phi(\mathbf{r}, \omega). \quad (5)$$

On substituting from (3) into (1) we obtain the following equation for ψ :

$$\nabla^2 \psi(\mathbf{r}, \omega) + [\nabla \psi(\mathbf{r}, \omega)]^2 = -k^2 n^2(\mathbf{r}, \omega). \quad (6)$$

* S. M. Rytov, *Izv. Akad. Nauk. SSSR, Ser. FIZ*, **2** (1937), 223.

This is a nonlinear equation which has the mathematical form of the so-called Riccati equation.

As in §13.1 we assume that the refractive index $n(\mathbf{r}, \omega)$ differs only slightly from unity so that

$$n(\mathbf{r}, \omega) = 1 + \delta n(\mathbf{r}, \omega), \quad (\delta n \ll 1). \quad (7)$$

It will be convenient to introduce a perturbation parameter μ which will facilitate keeping track of the powers of various terms in the perturbation expansion. We set

$$\delta n(\mathbf{r}) = \frac{1}{2}\mu\beta(\mathbf{r}). \quad (8)$$

The exact choice of μ is not crucial. It then follows from (7) and (8) that

$$n^2 \approx 1 + 2\delta n = 1 + \mu\beta, \quad (9)$$

and (6) becomes

$$\nabla^2 \psi(\mathbf{r}, \omega) + [\nabla \psi(\mathbf{r}, \omega)]^2 + k^2 + k^2 \mu \beta(\mathbf{r}) = 0. \quad (10)$$

The Liouville-Neumann series (see §13.1) may be expressed in the form

$$U(\mathbf{r}) = U^{(0)}(\mathbf{r}) + U^{(1)}(\mathbf{r}) + U^{(2)}(\mathbf{r}) + \cdots, \quad (11)$$

where $U^{(0)} \equiv U^{(i)}$ denotes the incident field, assumed to be a homogeneous plane wave or a linear superposition of such waves. $U^{(1)} \equiv U_1 - U_0$ is a term which is linear in the scattering potential $F(\mathbf{r})$, $U^{(2)} \equiv U_2 - U_1$ is quadratic in the scattering potential, etc (see §13.1.4). In the Rytov method, as already mentioned, one expands the $\psi(\mathbf{r})$ in a similar manner, viz.

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \mu\psi_1(\mathbf{r}) + \mu^2\psi_2(\mathbf{r}) + \cdots, \quad (12)$$

where ψ_1 is linear in F , ψ_2 is quadratic in F , etc. Expression (3) for the total field then becomes

$$U(\mathbf{r}) = e^{[\psi_0(\mathbf{r}) + \mu\psi_1(\mathbf{r}) + \mu^2\psi_2(\mathbf{r}) + \cdots]}, \quad (13)$$

known as the *Rytov expansion*.

One can readily obtain recurrence relations for the successive terms by substituting expansion (12) into the Riccati equation (10) and equating the groups of terms containing equal powers of the perturbation parameter μ . One then finds that

$$(\nabla^2 \psi_0) + (\nabla \psi_0)^2 = -k^2, \quad (14a)$$

$$\nabla^2 \psi_1 + 2\nabla \psi_0 \cdot \nabla \psi_1 = -k^2 \beta, \quad (14b)$$

$$\nabla^2 \psi_2 + 2\nabla \psi_0 \cdot \nabla \psi_2 = (\nabla \psi_1)^2, \quad (14c)$$

$$\nabla^2 \psi_3 + 2\nabla \psi_0 \cdot \nabla \psi_3 = -2(\nabla \psi_1) \cdot (\nabla \psi_2), \quad (14d)$$

$$\vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots$$

$$\nabla^2 \psi_n + 2\nabla \psi_0 \cdot \nabla \psi_n = - \sum_{k=1}^{n-1} \nabla \psi_k \cdot \nabla \psi_{n-k}. \quad (14e)$$

The first equation, (14a), is independent of the medium and hence ψ_0 must be associated with the incident field $U^{(i)}$, i.e.

$$e^{\psi_0(\mathbf{r}, \omega)} = U^{(i)}(\mathbf{r}, \omega). \quad (15)$$

The other equations are all of the form

$$\nabla^2 \psi_n + 2\nabla \psi_0 \cdot \nabla \psi_n = -g_n. \quad (16)$$

We note that the factor g_n on the right-hand side of (16) is known if all the preceding equations have been solved.

Eq. (16) may be reduced to a well-known form with the help of the substitution

$$\psi_n(\mathbf{r}, \omega) = e^{-\psi_0(\mathbf{r}, \omega)} W_n(\mathbf{r}, \omega). \quad (17)$$

By straightforward calculation we find that

$$\nabla \psi_n = (-W_n \nabla \psi_0 + \nabla W_n) e^{-\psi_0}, \quad (18)$$

$$\nabla^2 \psi_n = [W_n (\nabla \psi_0)^2 - 2\nabla W_n \cdot \nabla \psi_0 - W_n (\nabla^2 \psi_0) + \nabla^2 W_n] e^{-\psi_0}, \quad (19)$$

and, using these expressions and (14a), (16) reduces to

$$\nabla^2 W_n + k^2 W_n = -g_n e^{\psi_0}. \quad (20)$$

Eq. (20) is an inhomogeneous Helmholtz equation for W_n . Its solution may readily be obtained using Green's function techniques, just as we did in connection with §13.1 (9), but noting that the source term, i.e. the right-hand side of (20) is now known. The solution of (20), subject to the requirement that W_n behaves as an outgoing spherical wave at infinity, is then seen at once to be given by the integral

$$W_n(\mathbf{r}, \omega) = \frac{1}{4\pi} \int_V g_n(\mathbf{r}', \omega) e^{\psi_0(\mathbf{r}', \omega)} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r', \quad (21)$$

where $k = \omega/c$ and the integration extends over the scattering volume V . Recalling (17) we finally obtain for ψ_n the expression

$$\psi_n(\mathbf{r}, \omega) = \frac{1}{4\pi} e^{-\psi_0(\mathbf{r}, \omega)} \int_V g_n(\mathbf{r}', \omega) e^{\psi_0(\mathbf{r}', \omega)} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r'. \quad (22)$$

Returning to the Rytov expansion (13) and retaining only the first two terms in the exponent we have

$$U(\mathbf{r}, \omega) \approx U_1^{(R)}(\mathbf{r}, \omega) = e^{\psi_0(\mathbf{r}, \omega) + \psi_1(\mathbf{r}, \omega)}. \quad (23)$$

$U_1^{(R)}$ is known as the Rytov approximation or, more appropriately, as the first-order Rytov approximation. If we make use of (15) we see that

$$U_1^{(R)}(\mathbf{r}, \omega) = U^{(i)}(\mathbf{r}, \omega) e^{\psi_1(\mathbf{r}, \omega)}. \quad (24)$$

It turns out that ψ_1 may be expressed in a simple way in terms of the first Born approximation. To show this we note that according to (16) and (14b) $g_1 = k^2 \beta$ or, using (9), we see that $g_1 = k^2(n^2 - 1)$. Using this expression in the integrand in (22) and again using (15) we see that

$$\psi_1(\mathbf{r}, \omega) = [U^{(i)}(\mathbf{r}, \omega)]^{-1} \left\{ \frac{k^2}{4\pi} \int_V [n^2(\mathbf{r}', \omega) - 1] U^{(i)}(\mathbf{r}', \omega) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3r' \right\}. \quad (25)$$

The expression in the curly brackets on the right will be recognized as representing the scattered field in the first-order Born approximation, when an arbitrary field $U^{(i)}(\mathbf{r}, \omega)$ rather than a plane wave $\exp(ik\mathbf{s}_0 \cdot \mathbf{r})$ is incident on the scatterer (see §13.1 (22) and §13.1 (6)). If we denote this expression by $[U_1^{(s)}]^{(B)}$, (25) becomes

$$\psi_1(\mathbf{r}, \omega) = [U^{(i)}(\mathbf{r}, \omega)]^{-1} [U_1^{(s)}(\mathbf{r}, \omega)]^{(B)}, \quad (26)$$

which, together with (24), establishes a relationship between the first-order Rytov approximation and the first-order Born approximation.

The relative merits of the Born and the Rytov approximations of the same orders have been discussed in many publications but no clear consensus has been reached. It was shown, however,* that if the incident field is a single plane wave, the n th-order ($n \geq 1$) Rytov approximation is valid over a much longer propagation path than the n th-order Born approximation; but that this result does not hold with more general incident fields. The Born approximation then appears to have significant advantages.

13.6 Scattering of electromagnetic waves

We have so far considered the scattering of light by inhomogeneous media within the framework of the scalar theory. We will now discuss it on the basis of electromagnetic theory. However, because a full treatment is appreciably more involved and requires a much more extensive mathematical analysis, we will restrict ourselves to deriving only some of the more important results of the theory of static scattering of electromagnetic waves.†

13.6.1 The integro-differential equations of electromagnetic scattering theory

Let

$$\mathbf{E}^{(i)}(\mathbf{r}, t) = \mathcal{R}\{\mathbf{E}^{(i)}(\mathbf{r}, \omega)e^{-i\omega t}\}, \quad (1a)$$

$$\mathbf{H}^{(i)}(\mathbf{r}, t) = \mathcal{R}\{\mathbf{H}^{(i)}(\mathbf{r}, \omega)e^{-i\omega t}\}, \quad (1b)$$

(\mathcal{R} denoting the real part) represent the electric and the magnetic fields respectively of a monochromatic wave incident on a medium occupying a volume V in free space. We assume that the macroscopic properties of the medium do not change in time.

Under the influence of the incident field a polarization $\mathbf{P}(\mathbf{r}, t)$ and magnetization $\mathbf{M}(\mathbf{r}, t)$ will be induced in the medium. If the response of the medium is linear, $\mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t)$ will also oscillate with frequency ω , i.e. they will have the form

* J. B. Keller, *J. Opt. Soc. Amer.*, **59** (1969), 1003.

† For a discussion of dynamic scattering, i.e. scattering from media whose macroscopic response to an incident field is time-dependent, see N. G. van Kampen, in *Quantum Optics, Proceedings of the International School of Physics 'Enrico Fermi'*, Course XLII, Varenna, 1967, ed. R. J. Glauber (New York, Academic, 1969), p. 235; R. Pecora, *J. Chem. Phys.*, **40** (1964), 1604; E. Wolf and J. T. Foley, *Phys. Rev. A*, **40** (1989), 579; and B. J. Berne and R. Pecora, *Dynamic Light Scattering* (New York, J. Wiley and Sons, 1976).

$$\mathbf{P}(\mathbf{r}, t) = \mathcal{R}\{\mathbf{P}(\mathbf{r}, \omega)e^{-i\omega t}\}, \quad (2a)$$

$$\mathbf{M}(\mathbf{r}, t) = \mathcal{R}\{\mathbf{M}(\mathbf{r}, \omega)e^{-i\omega t}\}. \quad (2b)$$

A new field will then be generated whose electric and magnetic vectors may be expressed in the form (omitting from now on the time-dependent factor $\exp(-i\omega t)$ and also sometimes, for the sake of brevity, the argument ω)

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{(i)}(\mathbf{r}) + \mathbf{E}^{(s)}(\mathbf{r}), \quad (3a)$$

$$\mathbf{H}(\mathbf{r}) = \mathbf{H}^{(i)}(\mathbf{r}) + \mathbf{H}^{(s)}(\mathbf{r}), \quad (3b)$$

where $\mathbf{E}^{(s)}$ and $\mathbf{H}^{(s)}$ represent the scattered field.

For many media interacting with weak fields the constitutive relations which connect \mathbf{P} and \mathbf{M} with \mathbf{E} and \mathbf{H} have the form

$$\mathbf{P}(\mathbf{r}) = \eta(\mathbf{r})\mathbf{E}(\mathbf{r}), \quad \mathbf{M}(\mathbf{r}) = \chi(\mathbf{r})\mathbf{H}(\mathbf{r}), \quad (4)$$

where η is the dielectric susceptibility and χ is the magnetic permeability. In general both depend not only on \mathbf{r} but also on ω .

It follows from §2.2 (43), §2.2 (45), §2.2 (38) and §2.2 (39), specialized to monochromatic fields, that the total field (incident plus scattered) may be expressed in the form

$$\mathbf{E}(\mathbf{r}, \omega) = \mathbf{E}^{(i)}(\mathbf{r}, \omega) + \text{curl curl } \mathbf{\Pi}_e(\mathbf{r}, \omega) + ik \text{ curl } \mathbf{\Pi}_m(\mathbf{r}, \omega) - 4\pi\mathbf{P}(\mathbf{r}, \omega), \quad (5a)$$

$$\mathbf{H}(\mathbf{r}, \omega) = \mathbf{H}^{(i)}(\mathbf{r}, \omega) + \text{curl curl } \mathbf{\Pi}_m(\mathbf{r}, \omega) - ik \text{ curl } \mathbf{\Pi}_e(\mathbf{r}, \omega) - 4\pi\mathbf{M}(\mathbf{r}, \omega), \quad (5b)$$

where $\mathbf{\Pi}_e$ and $\mathbf{\Pi}_m$ are the electric and the magnetic Hertz potentials respectively, defined by the formulas

$$\mathbf{\Pi}_e(\mathbf{r}, \omega) = \int_V \mathbf{P}(\mathbf{r}', \omega) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r', \quad (6a)$$

$$\mathbf{\Pi}_m(\mathbf{r}, \omega) = \int_V \mathbf{M}(\mathbf{r}', \omega) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d^3 r'. \quad (6b)$$

When the polarization and magnetization in (5) and (6) are expressed in terms of the electric and the magnetic field vectors via the constitutive relations (4), Eqs. (5) become a pair of coupled integro-differential equations for the total fields \mathbf{E} and \mathbf{H} . After they have been solved for values of the field vectors at all points inside the scatterer, one can determine their values at any point outside the scattering volume V by substituting the solution for the interior points into (5), carrying out the integrations and applying the differential operators. We note that at points outside the scattering volume V , the terms $4\pi\mathbf{P}$ and $4\pi\mathbf{M}$ on the right-hand side of (5) have zero values.

The coupled pair of the integro-differential equations (5a) and (5b) are the analogues for electromagnetic scattering of the integral equation §13.1 (16) of the scalar theory of scattering (generalized to an arbitrary incident field).

13.6.2 The far field

In the majority of scattering experiments, measurements of the scattered field are made far away from the scatterer. We will, therefore, examine the behaviour of the scattered field in the far zone.

Let \mathbf{rs} ($s^2 = 1$) be the position vector of a point \mathbf{r} at a great distance from the scatterer. The spherical wave term in the integrands of expressions (6a) and (6b) for the Hertz potentials may then be approximated by the expression §13.1 (18) (see Fig. 13.3), viz.

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \sim \frac{e^{ikr}}{r} e^{-i\mathbf{k}\cdot\mathbf{r}'} \quad (7)$$

and the expressions (6a) and (6b) for the Hertz vectors take the form

$$\mathbf{\Pi}_e(\mathbf{rs}) \sim \tilde{\mathbf{P}}(k\mathbf{s}) \frac{e^{ikr}}{r}, \quad (8a)$$

$$\mathbf{\Pi}_m(\mathbf{rs}) \sim \tilde{\mathbf{M}}(k\mathbf{s}) \frac{e^{ikr}}{r}, \quad (8b)$$

where $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{M}}$ are the three-dimensional Fourier transforms of \mathbf{P} and of \mathbf{M} respectively, viz.

$$\tilde{\mathbf{P}}(\mathbf{k}) = \int_V \mathbf{P}(\mathbf{r}') e^{-i\mathbf{k}\cdot\mathbf{r}'} d^3 r', \quad (9a)$$

$$\tilde{\mathbf{M}}(\mathbf{k}) = \int_V \mathbf{M}(\mathbf{r}') e^{-i\mathbf{k}\cdot\mathbf{r}'} d^3 r'. \quad (9b)$$

Expressions (8) are the asymptotic approximations to $\mathbf{\Pi}_e(\mathbf{rs})$ and $\mathbf{\Pi}_m(\mathbf{rs})$ as $kr \rightarrow \infty$, with the direction \mathbf{s} being kept fixed. It follows from (8a) and (8b) on using elementary vector identities and retaining only terms in power of $1/r$ that

$$\text{curl } \mathbf{\Pi}_e(\mathbf{rs}) \sim ik[\mathbf{s} \times \tilde{\mathbf{P}}(k\mathbf{s})] \frac{e^{ikr}}{r}, \quad (10a)$$

$$\text{curl curl } \mathbf{\Pi}_e(\mathbf{rs}) \sim -k^2\{\mathbf{s} \times [\mathbf{s} \times \tilde{\mathbf{P}}(k\mathbf{s})]\} \frac{e^{ikr}}{r}. \quad (10b)$$

On substituting these expressions and similar expressions involving $\mathbf{\Pi}_m$ and $\tilde{\mathbf{M}}$ into (5) and recalling that $\mathbf{P}(\mathbf{r}) = 0$ and $\mathbf{M}(\mathbf{r}) = 0$ at points outside the scattering volume we obtain the following formulae for the electric and the magnetic fields in the far zone:

$$\mathbf{E}(\mathbf{rs}, \omega) \sim \mathbf{E}^{(i)}(\mathbf{rs}, \omega) - k^2\{\mathbf{s} \times [\mathbf{s} \times \tilde{\mathbf{P}}(k\mathbf{s}, \omega)] + \mathbf{s} \times \tilde{\mathbf{M}}(k\mathbf{s}, \omega)\} \frac{e^{ikr}}{r}, \quad (11a)$$

$$\mathbf{H}(\mathbf{rs}, \omega) \sim \mathbf{H}^{(i)}(\mathbf{rs}, \omega) - k^2\{\mathbf{s} \times [\mathbf{s} \times \tilde{\mathbf{M}}(k\mathbf{s}, \omega)] - \mathbf{s} \times \tilde{\mathbf{P}}(k\mathbf{s}, \omega)\} \frac{e^{ikr}}{r}. \quad (11b)$$

It follows that the scattered field in the far zone may be expressed in the form

$$\mathbf{E}^{(s)}(\mathbf{rs}, \omega) \sim \mathbf{A}(\mathbf{s}, \omega) \frac{e^{ikr}}{r}, \quad (12a)$$

$$\mathbf{H}^{(s)}(\mathbf{rs}, \omega) \sim \mathbf{s} \times \mathbf{A}(\mathbf{s}, \omega) \frac{e^{ikr}}{r}, \quad (12b)$$

where

$$\mathbf{A}(\mathbf{s}, \omega) = -k^2 \{ \mathbf{s} \times [\mathbf{s} \times \tilde{\mathbf{P}}(k\mathbf{s}, \omega)] + \mathbf{s} \times \tilde{\mathbf{M}}(k\mathbf{s}, \omega) \}. \quad (13)$$

It is evident from (13) that $\mathbf{s} \cdot \mathbf{A}(\mathbf{s}, \omega) = 0$, i.e. that the vector $\mathbf{A}(\mathbf{s}, \omega)$ is orthogonal to \mathbf{s} ; and we also see from (12) that in the far zone the vectors $\mathbf{E}^{(s)}$, $\mathbf{H}^{(s)}$ and \mathbf{s} form an orthogonal triad of vectors which is right-handed in that order (see Fig. 13.16). Moreover, $\mathbf{E}^{(s)}(r\mathbf{s})$ and $\mathbf{H}^{(s)}(r\mathbf{s})$ have the same magnitude. Hence, at each point in the far zone the scattered electromagnetic field has the structure of a plane electromagnetic wave which propagates in the direction of the unit vector \mathbf{s} , i.e. in the outward radial direction from the scatterer. We also see from (12) that the overall behaviour of the far field is that of an outgoing spherical wave.

The values of $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{M}}$ in (13), just like the values of \mathbf{P} and \mathbf{M} which appear in (6), depend on the values of the field vectors \mathbf{E} and \mathbf{H} which can only be obtained by solving the coupled set of the integro-differential equations (5a) and (5b). However, if the scattering is sufficiently weak we may approximate \mathbf{P} and \mathbf{M} by neglecting contributions of the scattered field on the right-hand side of the constitutive relations (4), i.e. we may then approximate \mathbf{P} by $\eta \mathbf{E}^{(i)}$ and \mathbf{M} by $\chi \mathbf{H}^{(i)}$. The resulting expressions for \mathbf{E} and \mathbf{H} which are then obtained from (5) are evidently the analogues of §13.1 (22) for the field in the scalar theory of scattering, calculated within the accuracy of the first-order Born approximation (with an arbitrary incident field rather than with the plane wave $\exp(ik\mathbf{s}_0 \cdot \mathbf{r})$).

13.6.3 The optical cross-section theorem for scattering of electromagnetic waves

In §13.3 we discussed within the framework of scalar wave theory the so-called optical cross-section theorem. It expresses the rate at which energy is removed from an incident plane wave by the process of scattering and absorption in terms of the forward scattering amplitude. We will now derive a corresponding theorem for scattering of electromagnetic waves.

Consider a plane monochromatic wave incident on an obstacle of arbitrary form. The field at any point in the medium surrounding the obstacle may again be represented as the sum of the incident field and the scattered field

$$\mathbf{E} = \mathbf{E}^{(i)} + \mathbf{E}^{(s)}, \quad \mathbf{H} = \mathbf{H}^{(i)} + \mathbf{H}^{(s)}. \quad (14)$$

As usual, we omit a time-dependent factor $\exp(-i\omega t)$. The time-averaged energy flux

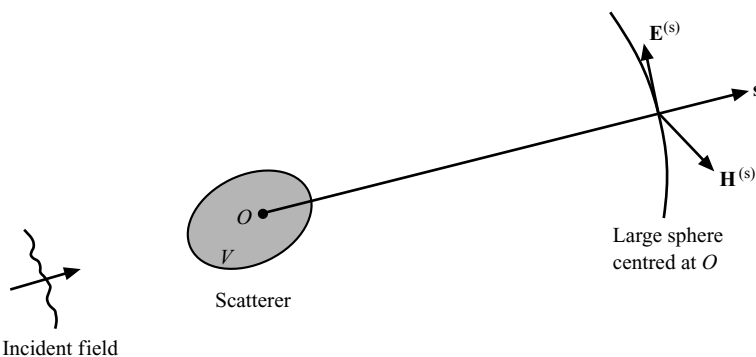


Fig. 13.16 Illustrating the behaviour of the scattered electromagnetic field $\mathbf{E}^{(s)}$, $\mathbf{H}^{(s)}$ in the far zone.

is represented by the time-averaged Poynting vector which, according to (14) and §1.4 (56) is given by

$$\langle \mathbf{S} \rangle = \langle \mathbf{S}^{(i)} \rangle + \langle \mathbf{S}^{(s)} \rangle + \langle \mathbf{S}' \rangle, \quad (15)$$

where (\mathcal{R} denoting the real part)

$$\langle \mathbf{S}^{(i)} \rangle = \frac{c}{8\pi} \mathcal{R} \{ \mathbf{E}^{(i)} \times \mathbf{H}^{(i)\star} \}, \quad (16a)$$

$$\langle \mathbf{S}^{(s)} \rangle = \frac{c}{8\pi} \mathcal{R} \{ \mathbf{E}^{(s)} \times \mathbf{H}^{(s)\star} \}, \quad (16b)$$

$$\langle \mathbf{S}' \rangle = \frac{c}{8\pi} \mathcal{R} \{ \mathbf{E}^{(i)} \times \mathbf{H}^{(s)\star} + \mathbf{E}^{(s)} \times \mathbf{H}^{(i)\star} \}. \quad (16c)$$

Consider the averaged outward flow of energy through the surface of a large sphere of radius R , centred at some point in the region occupied by the obstacle. The net flow per second is represented by the integral of the radial component $\langle \mathbf{S} \rangle_r$ of $\langle \mathbf{S} \rangle$, taken over the sphere, and is evidently zero when the obstacle is a dielectric. If, however, the obstacle is a conductor, some of the incident energy is absorbed by it and the net outward flow through the surface of the sphere is equal in magnitude to the rate at which absorption takes place. Let $\mathcal{W}^{(a)}$ be the rate at which the energy is being absorbed by the obstacle. Then, from (15)

$$-\mathcal{W}^{(a)} = \mathcal{W}^{(i)} + \mathcal{W}^{(s)} + \mathcal{W}', \quad (17)$$

where $\mathcal{W}^{(i)}$, $\mathcal{W}^{(s)}$ and \mathcal{W}' are the integrals of the radial components $\langle \mathbf{S}^{(i)} \rangle_r$, $\langle \mathbf{S}^{(s)} \rangle_r$, and $\langle \mathbf{S}' \rangle_r$ over the surface of the sphere respectively. One can readily show by analogy with the discussion leading to §13.3 (11) for the scalar case that $\mathcal{W}^{(i)} = 0$, so that

$$\mathcal{W}^{(a)} + \mathcal{W}^{(s)} = -\mathcal{W}' = -\frac{c}{8\pi} \mathcal{R} \iint_{\Sigma} \{ \mathbf{E}^{(i)} \times \mathbf{H}^{(s)\star} + \mathbf{E}^{(s)} \times \mathbf{H}^{(i)\star} \} \cdot \mathbf{n} \, dS, \quad (18)$$

S denoting the large sphere and \mathbf{n} the unit outward normal. Thus the expression on the right of (18) represents the rate at which energy is dissipated by heat and by scattering.

Let \mathbf{s}_0 be the unit vector in the direction in which the incident wave propagates so that

$$\mathbf{E}^{(i)} = \mathbf{e} e^{ik(\mathbf{s}_0 \cdot \mathbf{r})}, \quad \mathbf{H}^{(i)} = \mathbf{h} e^{ik(\mathbf{s}_0 \cdot \mathbf{r})}. \quad (19)$$

We assume that this wave is linearly polarized, so that \mathbf{e} and \mathbf{h} may be assumed to be real unit vectors. At a large distance from the obstacle the scattered wave is spherical (see (12)):

$$\mathbf{E}^{(s)} = \mathbf{a}(\mathbf{s}) \frac{e^{ikr}}{r}, \quad \mathbf{H}^{(s)} = \mathbf{b}(\mathbf{s}) \frac{e^{ikr}}{r}. \quad (20)$$

The vectors $\mathbf{a}(\mathbf{s})$ and $\mathbf{b}(\mathbf{s})$ characterize the strength of the radiation scattered in the direction \mathbf{s} . Since the incident and scattered waves obey Maxwell's equations we have (§1.4 (4), §1.4 (5), with $\varepsilon = \mu = 1$)

$$\left. \begin{aligned} \mathbf{h} &= \mathbf{s}_0 \times \mathbf{e}, & \mathbf{b} &= \mathbf{s} \times \mathbf{a}, \\ \mathbf{s}_0 \cdot \mathbf{e} &= \mathbf{s}_0 \cdot \mathbf{h} = 0, & \mathbf{s} \cdot \mathbf{a} &= \mathbf{s} \cdot \mathbf{b} = 0. \end{aligned} \right\} \quad (21)$$

From these relations it follows that on the surface of the large sphere Σ ,

$$\left. \begin{aligned} (\mathbf{E}^{(i)} \times \mathbf{H}^{(s)\star}) \cdot \mathbf{s} &= \mathbf{e} \cdot \mathbf{a}^\star(\mathbf{s}) e^{ikR(\mathbf{s}_0 \cdot \mathbf{s})} \frac{e^{-ikR}}{R}, \\ (\mathbf{E}^{(s)} \times \mathbf{H}^{(i)\star}) \cdot \mathbf{s} &= \{(\mathbf{s} \cdot \mathbf{s}_0)[\mathbf{a}(\mathbf{s}) \cdot \mathbf{e}] - (\mathbf{s} \cdot \mathbf{e})[\mathbf{s}_0 \cdot \mathbf{a}(\mathbf{s})]\} e^{-ikR(\mathbf{s}_0 \cdot \mathbf{s})} \frac{e^{ikR}}{R}, \end{aligned} \right\} \quad (22)$$

where we used the fact that $\mathbf{n} = \mathbf{s}$ on the large sphere Σ . We substitute these expressions in (18). The resulting integral may be evaluated by the use of Jones' lemma (§13.3 (15)). We then find that

$$\left. \begin{aligned} \iint_{\Sigma} (\mathbf{E}^{(i)} \times \mathbf{H}^{(s)\star}) \cdot \mathbf{n} \, dS &\sim -\frac{2\pi i}{k} [\mathbf{e} \cdot \mathbf{a}^\star(\mathbf{s}_0) - \mathbf{e} \cdot \mathbf{a}^\star(-\mathbf{s}_0) e^{-2ikR}], \\ \iint_{\Sigma} (\mathbf{E}^{(s)} \times \mathbf{H}^{(i)\star}) \cdot \mathbf{n} \, dS &\sim -\frac{2\pi i}{k} [\mathbf{e} \cdot \mathbf{a}(\mathbf{s}_0) + \mathbf{e} \cdot \mathbf{a}(-\mathbf{s}_0) e^{2ikR}], \end{aligned} \right\} \quad (23)$$

and (18) becomes

$$\mathcal{W}^{(s)} + \mathcal{W}^{(a)} = \frac{c}{2k} \mathcal{I}[\mathbf{e} \cdot \mathbf{a}(\mathbf{s}_0)], \quad (24)$$

where \mathcal{I} denotes the imaginary part.

Relation (24) implies that *with incident light that is linearly polarized, the rate at which the energy is dissipated is proportional to a certain amplitude component of the scattered wave; the amplitude is that which corresponds to forward scattering ($\mathbf{s} = \mathbf{s}_0$) and the component is in the direction of the electric vector of the incident wave.*

As in the case of scalar scattering the ratio Q between the rate of dissipation of energy ($\mathcal{W}^{(a)} + \mathcal{W}^{(s)}$) and the rate at which the energy is incident on a unit cross-sectional area of the obstacle $|\langle \mathbf{S}^{(i)} \rangle|$ is called the *extinction cross-section* of the obstacle. From (16a), (19) and (21) it follows that $|\langle \mathbf{S}^{(i)} \rangle| = c\mathbf{e}^2/8\pi$ so that we have, according to (24),

$$Q = \frac{\mathcal{W}^{(s)} + \mathcal{W}^{(a)}}{|\langle \mathbf{S}^{(i)} \rangle|} = \frac{4\pi}{k} \mathcal{I} \left\{ \frac{\mathbf{e} \cdot \mathbf{a}(\mathbf{s}_0)}{\mathbf{e}^2} \right\}. \quad (25)$$

The formula (25) expresses the *optical cross-section theorem* for scattering of electromagnetic waves.

One may define the *scattering cross-section* $Q^{(s)}$ and the *absorption cross-section* $Q^{(a)}$ of the obstacle in a similar way:

$$Q^{(s)} = \frac{\mathcal{W}^{(s)}}{|\langle \mathbf{S}^{(i)} \rangle|}, \quad Q^{(a)} = \frac{\mathcal{W}^{(a)}}{|\langle \mathbf{S}^{(i)} \rangle|}, \quad (26)$$

and evidently $Q = Q^{(s)} + Q^{(a)}$. For a nonabsorbing obstacle $Q^{(a)} = 0$ and the extinction cross-section is then equal to the scattering cross-section.