

# Chapter 1

## Introducing Reflection

Electromagnetic, acoustic and particle waves all scatter, diffract and interfere. Reflection is the result of the constructive interference of many scattered or diffracted waves originating from scatterers in a stratified medium. This fundamental many-body approach is hard to apply (two illustrations are given in Sect. 1.5). Usually one replaces the collection of scatterers by an effective medium whose properties are represented, as far as wave propagation is concerned, by a function of position and frequency (or energy), such as the dielectric function  $\varepsilon$  in the electromagnetic case, or the effective potential  $V$  in the quantum particle case. Electromagnetic and particle waves then satisfy the same kind of linear partial differential equation, with  $\varepsilon$  and  $V$  playing similar roles.

In a medium with planar stratification the functions  $\varepsilon$  and  $V$  depend on only one spatial variable, and the partial differential equations then separate. Snell's Law is a direct consequence of this separability of the spatial dependence, or equivalently, of the invariance of the reflecting material with respect to translations along the surface. The differential equations, and the elementary reflection properties which follow from them, are derived for electromagnetic, particle, and acoustic waves in the first four sections. The many-body, constructive interference, aspect of reflection is outlined in Sect. 1.5. Finally, Sect. 1.6 previews some of the main results in Chaps. 2–20.

### 1.1 The Electromagnetic $s$ Wave

The reflection of a plane electromagnetic wave at a planar interface between two media is completely characterized when solutions for two mutually perpendicular polarizations are known. The polarizations conventionally chosen are: one with its electric vector perpendicular to the plane of incidence (labelled  $s$ , from the German *senkrecht*, perpendicular), and the other with its electric vector parallel to the plane of incidence (labelled  $p$ ).

We consider monochromatic waves, of angular frequency  $\omega$ . The reflection of a general electromagnetic wave (a pulse, for example) can be analysed as that of a superposition of monochromatic waves. For a given  $\omega$  the time dependence of all

fields is carried in the factor  $e^{-i\omega t}$ . (This is the convention in quantum and solid state physics, and much of optics. In radio and electrical engineering the factor  $e^{i\omega t}$  is often used. With the convention used here the dielectric function has positive imaginary part in the case of absorption.) We will mostly consider *non-magnetic* media in this book. The electrodynamic properties of a medium are then contained in the dielectric function  $\varepsilon(\mathbf{r}, \omega)$  which is the ratio of the permittivity of the medium at position  $\mathbf{r}$  and angular frequency  $\omega$  to that of the vacuum. The wave equations follow from Maxwell's two curl equations relating the electric field  $\mathbf{E}$  and the magnetic field  $\mathbf{B}$ :

$$\nabla \times \mathbf{E} = i\omega\mathbf{B} \quad \text{or} \quad \nabla \times \mathbf{E} = i\frac{\omega}{c}\mathbf{B}, \quad (1.1)$$

$$\nabla \times \mathbf{B} = -i\varepsilon\frac{\omega}{c^2}\mathbf{E} \quad \text{or} \quad \nabla \times \mathbf{B} = -i\varepsilon\frac{\omega}{c}\mathbf{E}. \quad (1.2)$$

(The equations on the left are in SI units, those on the right in Gaussian units; the difference lies in the positioning of the speed of light  $c$ . In reflection studies, theory and experiment deal in dimensionless ratios, which are independent of the choice of units. Even the formal distinction disappears from (1.5) onward.)

For a planar interface lying in the  $xy$  plane, and an electromagnetic wave propagating in the  $x$  and  $z$  directions, the  $s$  wave has  $\mathbf{E} = (0, E_y, 0)$  and (1.1) gives

$$-\frac{\partial E_y}{\partial z} = i\frac{\omega}{c}B_x, \quad \frac{\partial E_y}{\partial x} = i\frac{\omega}{c}B_z, \quad (1.3)$$

and  $B_y = 0$ . The other curl equation gives

$$\frac{\partial B_x}{\partial z} - \frac{\partial B_z}{\partial x} = -i\varepsilon\frac{\omega}{c}E_y. \quad (1.4)$$

On eliminating  $B_x$  and  $B_z$  from (1.3) and (1.4), we obtain a second order partial differential equation for  $E_y$ ,

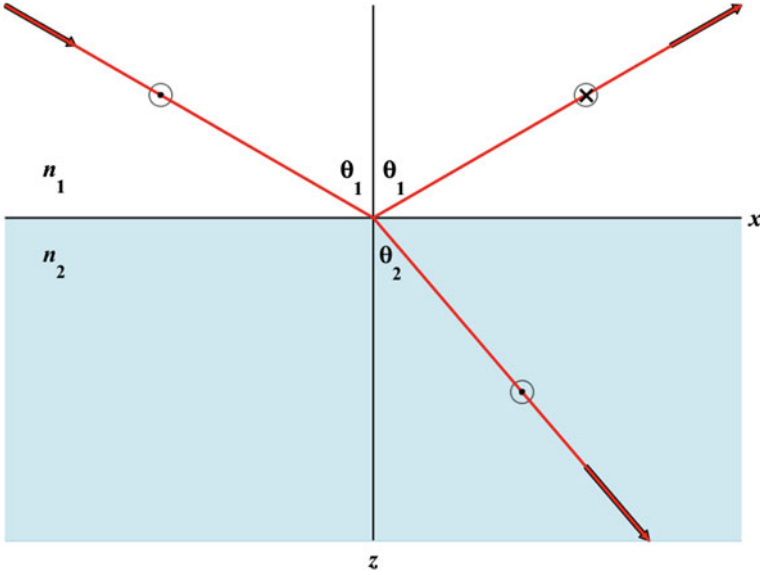
$$\frac{\partial^2 E_y}{\partial x^2} + \frac{\partial^2 E_y}{\partial z^2} + \varepsilon\frac{\omega^2}{c^2}E_y = 0. \quad (1.5)$$

For planar stratifications the dielectric function depends on one spatial variable,  $z$ . The partial differential equation is then separable, with

$$E_y(x, z, t) = e^{i(Kx - \omega t)}E(z), \quad (1.6)$$

where  $E(z)$  satisfies the ordinary differential equation

$$\frac{d^2 E}{dz^2} + q^2 E = 0, \quad q^2 = \varepsilon\frac{\omega^2}{c^2} - K^2 = k^2 - K^2. \quad (1.7)$$



**Fig. 1.1** Reflection of the electromagnetic  $s$  wave at a planar interface between media characterized by dielectric constants  $\epsilon_1 = n_1^2$  and  $\epsilon_2 = n_2^2$ . The figure is drawn the air|water interface at optical frequencies, with  $\epsilon_1 \approx 1$ ,  $\epsilon_2 \approx (4/3)^2$

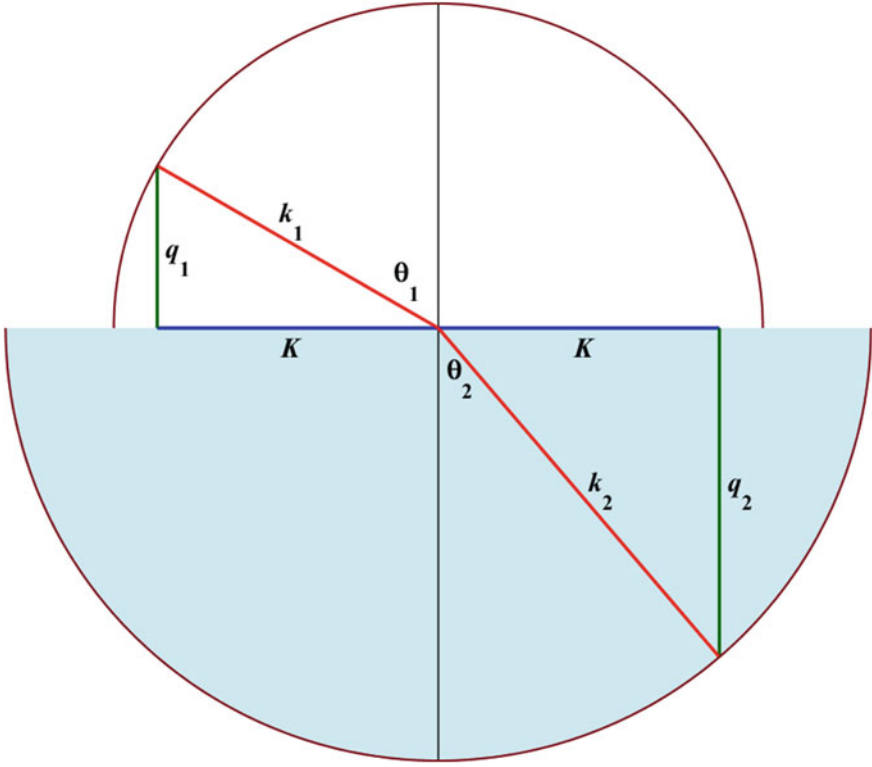
The meanings of  $k$ ,  $K$  and  $q$  are evident from (1.5), (1.6) and (1.7):  $k = \epsilon^{1/2}\omega/c$  is the local magnitude of the wavevector,  $K = k_x$  is the component of the wavevector along the interface, and  $q = k_z$  is the component of the wavevector normal to the interface. For a plane wave incident from medium 1 as shown in Fig. 1.1, the existence of the separation-of-variables constant  $K (= k_{1x} = k'_{1x} = k_{2x})$  implies

$$\epsilon_1^{1/2} \sin \theta_1 = \epsilon_1^{1/2} \sin \theta'_1 = \epsilon_2^{1/2} \sin \theta_2, \quad (1.8)$$

where  $\theta_1$ ,  $\theta'_1$ , and  $\theta_2$  are the angles of incidence, reflection, and transmission (or refraction).

Thus the fact that  $\epsilon$  is a function of one spatial coordinate only, and the consequent separation of variables, implies the laws of reflection and refraction: the angle of reflection is equal to the angle of incidence, and the angles of incidence and refraction are related by Snell's Law. The refractive indices of the two media, defined as coefficients in Snell's Law  $n_1 \sin \theta_1 = n_2 \sin \theta_2$ , are  $n_1 = \sqrt{\epsilon_1}$  and  $n_2 = \sqrt{\epsilon_2}$ . Note that the laws of reflection-refraction do not depend on the transition between the two media being sharp: they are valid for an arbitrary variation of  $\epsilon(z)$  between the asymptotic values  $\epsilon_1$  and  $\epsilon_2$ .

As  $\epsilon$  attains its limiting values  $\epsilon_1 = n_1^2$  and  $\epsilon_2 = n_2^2$ ,  $q = (\epsilon\omega^2/c^2 - K^2)^{1/2}$  takes the limiting values



**Fig. 1.2** Graphical representation of  $k^2 = q^2 + K^2$  and  $K = k_1 \sin \theta_1 = k_2 \sin \theta_2$ . The figure is drawn for the air|water interface, as in Fig. 1.1. For incidence from the optically denser lower medium, as the angle of incidence  $\theta_2$  increases the magnitude of the tangential component  $K$  of the wavevector will increase beyond the magnitude  $k_1$  of the wavevector in the upper medium. No transmitted wave is then possible, and there will be total internal reflection

$$q_1 = n_1 \frac{\omega}{c} \cos \theta_1, \quad q_2 = n_2 \frac{\omega}{c} \cos \theta_2. \quad (1.9)$$

(For  $\theta_1 > \theta_c = \arcsin(n_2/n_1)$  there is total reflection,  $q_2$  is imaginary, and  $\theta_2$  is complex. This is discussed along with the particle case in Sect. 1.3.) Snell's Law and the relationships between the wavevector components are incorporated together in Fig. 1.2.

We now define the reflection and transmission amplitudes  $r_s$  and  $t_s$  in terms of the limiting forms of the solution of (1.7):

$$e^{iq_1 z} + r_s e^{-iq_1 z} \leftarrow E(z) \rightarrow t_s e^{iq_2 z}. \quad (1.10)$$

The reflection amplitude is thus defined as the ratio of the coefficient of  $e^{-iq_1 z}$  to that of  $e^{iq_1 z}$ , the transmission amplitude as the coefficient of  $e^{iq_2 z}$  when the incident wave

$e^{iq_1 z}$  has unit amplitude. Theory aims to obtain general properties of the reflection and transmission amplitudes, and to develop methods for calculating these for a given dielectric function profile. The calculation is simple for the important *step profile*

$$\varepsilon_0(z) = \begin{cases} \varepsilon_1 & (z < 0) \\ \varepsilon_2 & (z > 0) \end{cases} \quad (1.11)$$

For this profile we obtain  $r_s$  and  $t_s$  from the continuity of  $E$  and  $dE/dz$  at  $z = 0$ . (If, for example,  $dE/dz$  were discontinuous,  $d^2E/dz^2$  would have a delta function part, and (1.7) would not be satisfied.) For the step profile,  $E$  is given by the left and right sides of (1.10) for  $z < 0$  and  $z > 0$ , respectively. The continuity of  $E$  and  $dE/dz$  at the origin gives

$$1 + r_{s0} = t_{s0}, \quad iq_1(1 - r_{s0}) = iq_2 t_{s0}. \quad (1.12)$$

Thus

$$r_{s0} = \frac{q_1 - q_2}{q_1 + q_2}, \quad t_{s0} = \frac{2q_1}{q_1 + q_2}. \quad (1.13)$$

On using (1.8) and (1.9), the expressions (1.13) may be put into the Fresnel forms (Fresnel 1823)

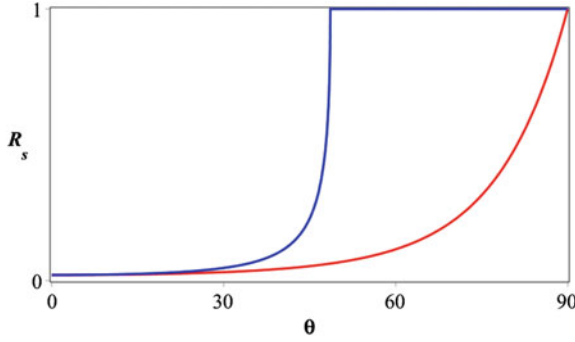
$$r_{s0} = \frac{\sin(\theta_2 - \theta_1)}{\sin(\theta_2 + \theta_1)}, \quad t_{s0} = \frac{2 \sin \theta_2 \cos \theta_1}{\sin(\theta_2 + \theta_1)} \quad (1.14)$$

The phases of the reflected and transmitted waves are specified only when the phase of the incident wave *and* the location of the interface are specified. The above equations are for the discontinuity in  $\varepsilon(z)$  located at  $z = 0$ . In general, for the step located at  $z_1$ ,

$$r_{s0} = e^{2iq_1 z_1} \frac{q_1 - q_2}{q_1 + q_2}, \quad t_{s0} = e^{i(q_1 - q_2)z_1} \frac{2q_1}{q_1 + q_2}. \quad (1.15)$$

A special situation arises at grazing incidence ( $\theta_1 \rightarrow \pi/2, q_1 \rightarrow 0$ ), when the incident and reflected waves are propagating in the same direction. Then the phase of the reflected wave is well-defined without specification of the interface location, and  $r_{s0} \rightarrow -1$  (even in the case of the total internal reflection, when  $q_2$  is imaginary). The fact that  $r_s \rightarrow -1$  at grazing incidence is a general property of reflection from all interfaces, as will be shown in Sect. 2.3.

The classical electromagnetic fields  $\mathbf{E}$  and  $\mathbf{B}$  are real quantities, and the complex notation is used for mathematical convenience. (Complex fields are intrinsic in the quantum theory of particles, however.) The physical reflected  $s$  wave is, for unit amplitude of the incident wave,



**Fig. 1.3** Step profile reflectivity for the  $s$  wave. The parameters are for the air|water interface at optical frequencies, as in Figs. 1.1 and 1.2. The *lower curve* is for light incident from air; the *upper curve* for light incident from water shows total internal reflection for angle of incidence greater than  $\theta_c = \arcsin(\frac{3}{4}) \approx 48.6^\circ$

$$\operatorname{Re}\{r_s e^{i(Kx - q_1 z - \omega t)}\} = \operatorname{Re}(r_s) \cos(Kx - q_1 z - \omega t) - \operatorname{Im}(r_s) \sin(Kx - q_1 z - \omega t)$$

The reflected intensity is proportional to the time average of the square of this, namely

$$\frac{1}{2} [\operatorname{Re}(r_s)]^2 + \frac{1}{2} [\operatorname{Im}(r_s)]^2 = \frac{1}{2} |r_s|^2$$

The incident intensity is proportional to the time average of  $\cos^2(Kx + q_1 z - \omega t)$ , which is  $1/2$ . Thus,  $R_s = |r_s|^2$  is the ratio of the reflected intensity to the incident intensity. This quantity is called the reflectivity, or reflectance. Figure 1.3 shows  $R_s$  for a sharp transition between air and water, with light incident from air, and from water.

## 1.2 The Electromagnetic $p$ Wave

We again take the incident and reflected waves propagating in the  $zx$  plane, and the stratifications lying in  $xy$  planes. For the  $p$  wave,  $\mathbf{B} = (0, B_y, 0)$ ; the Maxwell equation (1.1) gives

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = i \frac{\omega}{c} B_y, \quad (1.16)$$

while (1.2) implies  $E_y = 0$  and

$$\frac{\partial B_y}{\partial z} = i\varepsilon \frac{\omega}{c} E_x, \quad \frac{\partial B_y}{\partial x} = -i\varepsilon \frac{\omega}{c} E_z. \quad (1.17)$$

Elimination of  $E_x$  and  $E_z$  gives

$$\frac{\partial}{\partial x} \left( \frac{1}{\varepsilon} \frac{\partial B_y}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{1}{\varepsilon} \frac{\partial B_y}{\partial z} \right) + \frac{\omega^2}{c^2} B_y = 0. \quad (1.18)$$

When  $\varepsilon$  is a function of one spatial coordinate  $z$ , the laws of reflection and refraction again follow from the separability of (1.18). We set

$$B_y(x, z, t) = e^{i(Kx - \omega t)} B(z) \quad (1.19)$$

where  $K$  has the same meaning as for the  $s$  wave; then  $B(z)$  satisfies the ordinary differential equation

$$\frac{d}{dz} \left( \frac{1}{\varepsilon} \frac{dB}{dz} \right) + \left( \frac{\omega^2}{c^2} - \frac{K^2}{\varepsilon} \right) B = 0 \quad (1.20)$$

When  $\varepsilon$  is constant (outside the interfacial region), the  $p$  wave equation has the same form as the  $s$  wave equation, with the same wavevector component  $q$  perpendicular to the interface. But within the interface there is an additional term proportional to the product of  $d\varepsilon/dz$  and  $dB/dz$ . This term may be removed (and (1.20) converted to the form of the  $s$  wave (1.7)) in two ways. The first involves defining a new dependent variable

$$b = \left( \frac{\varepsilon_1}{\varepsilon} \right)^{1/2} B \quad (1.21)$$

(The factor  $\varepsilon_1^{1/2}$  makes identical the limiting forms of  $b$  and  $B$  in medium 1.) The equation satisfied by  $b$  is

$$\frac{d^2 b}{dz^2} + q_b^2 b = 0, \quad q_b^2 = q^2 - \varepsilon^{1/2} \frac{d^2 \varepsilon^{-1/2}}{dz^2} = q^2 + \frac{1}{2\varepsilon} \frac{d^2 \varepsilon}{dz^2} - \frac{3}{4} \left( \frac{1}{\varepsilon} \frac{d\varepsilon}{dz} \right)^2 \quad (1.22)$$

This form of the  $p$  polarization equation is useful for special profiles, in particular the exponential profile, which has  $\ln \varepsilon$  linear in  $z$ , and the Rayleigh profile, which has  $\varepsilon^{-1/2}$  linear in  $z$ . These are discussed in Chap. 2. It is also useful at short wavelengths, in the derivation of a perturbation theory for the  $p$  wave (Chap. 6).

The second transformation which removes the  $(d\varepsilon/dz)(dB/dz)$  term is a dilation of the  $z$  variable in proportion to the local value of  $\varepsilon(z)$ : we define a new independent variable  $Z$  by

$$dZ = \varepsilon dz \quad (1.23)$$

Then, as may be seen on division of (1.20) by  $\varepsilon$ , the  $p$  wave equation reads

$$\frac{d^2 B}{dZ^2} + Q^2 B = 0, \quad Q^2 = \frac{1}{\varepsilon} \frac{\omega^2}{c^2} - \frac{K^2}{\varepsilon^2} = \left(\frac{q}{\varepsilon}\right)^2. \quad (1.24)$$

This equation, in terms of the dilated  $z$  variable, and a reduced normal component of the wavevector,  $Q = q/\varepsilon$ , will be useful in many applications throughout this book.

The  $p$  wave reflection and transmission amplitudes are defined in terms of the limiting forms of  $B(z)$ :

$$e^{iq_1 z} - r_p e^{-iq_1 z} \leftarrow B(z) \rightarrow \frac{n_2}{n_1} t_p e^{iq_2 z} \quad (1.25)$$

The reason for the factors  $-1$  and  $n_2/n_1 = (\varepsilon_2/\varepsilon_1)^{1/2}$  multiplying  $r_p$  and  $t_p$  is that we wish  $r_s$  and  $r_p$  and  $t_p$  and  $t_s$  to refer to the same quantity, here chosen to be the electric field. (This is not the only convention in use: some authors have the opposite sign on  $r_p$ .) The electric field components for the  $p$  wave are found from (1.2), (1.19) and (1.25) to have the limiting forms

$$\varepsilon_1^{-1/2} \cos \theta_1 e^{i(Kx - \omega t)} (e^{iq_1 z} + r_p e^{-iq_1 z}) \leftarrow E_x \rightarrow \varepsilon_1^{-1/2} \cos \theta_2 t_p e^{i(Kx + q_2 z - \omega t)}, \quad (1.26)$$

$$-\varepsilon_1^{-1/2} \sin \theta_1 e^{i(Kx - \omega t)} (e^{iq_1 z} - r_p e^{-iq_1 z}) \leftarrow E_z \rightarrow -\varepsilon_1^{-1/2} \sin \theta_2 t_p e^{i(Kx + q_2 z - \omega t)}. \quad (1.27)$$

The  $x$ -component of the electric field (tangential to the interface) thus has the reflection amplitude  $r_p$ , while the  $z$ -component (normal to the interface) has reflection amplitude  $-r_p$ .

At normal incidence there is no physical difference between the  $s$  and  $p$  polarizations: both have electric and magnetic fields tangential to the interface. For our geometry,  $E_z$  is zero at normal incidence, and (1.1) implies  $\partial E_x / \partial z = i(\omega/c) B_y$ . Thus  $B$ , the solution of (1.20) and (1.25), must be proportional to  $dE/dz$ , where  $E$  is the solution of (1.7) and (1.10). On substituting  $dE/dz$  for  $B$  in (1.20) (with  $K$  set equal to zero) the left side becomes

$$\frac{d}{dz} \left\{ \frac{1}{\varepsilon} \left( \frac{d^2 E}{dz^2} + \varepsilon \frac{\omega^2}{c^2} E \right) \right\}$$

and this is zero, by (1.7). Thus (1.20) is satisfied by  $dE/dz$  at normal incidence. The proportionality of  $B$  and  $dE/dz$  at normal incidence, when applied to the limiting forms (1.10) and (1.25), gives the equality of  $r_p$  with  $r_s$  and of  $t_p$  with  $t_s$ .

(Proportionality of  $B$  and  $dE/dz$  could be replaced by equality of  $B$  and  $(c/i\omega)dE/dz$ , but then (1.25) would have to be modified by the factor  $n_1$ .)

At a discontinuity in the dielectric function,  $B$  and  $\varepsilon^{-1}dB/dz = dB/dZ$  are continuous (from (1.20) or (1.24)). For the step profile  $\varepsilon_0(z)$  defined by (1.11),  $B$  is equal to

$$B_0(z) = \begin{cases} e^{iq_1 z} - r_{p0} e^{-iq_1 z} & (z < 0) \\ \frac{n_2}{n_1} t_{p0} e^{iq_2 z} & (z > 0) \end{cases} \quad (1.28)$$

The continuity of  $B$  and  $\varepsilon^{-1}dB/dz$  at the origin gives

$$1 - r_{p0} = \frac{n_2}{n_1} t_{p0}, \quad (1.29)$$

$$iQ_1(1 + r_{p0}) = iQ_2 \frac{n_2}{n_1} t_{p0}, \quad (1.30)$$

where  $Q_1 = q_1/\varepsilon_1$  and  $Q_2 = q_2/\varepsilon_2$ . Thus (compare (1.13))

$$-r_{p0} = \frac{Q_1 - Q_2}{Q_1 + Q_2}, \quad \frac{n_2}{n_1} t_{p0} = \frac{2Q_1}{Q_1 + Q_2}. \quad (1.31)$$

On using (1.8) and (1.9) we obtain the Fresnel forms

$$r_{p0} = \frac{\tan(\theta_2 - \theta_1)}{\tan(\theta_2 + \theta_1)}, \quad t_{p0} = \frac{2 \sin \theta_2 \cos \theta_1}{\sin(\theta_2 + \theta_1) \cos(\theta_2 - \theta_1)} \quad (1.32)$$

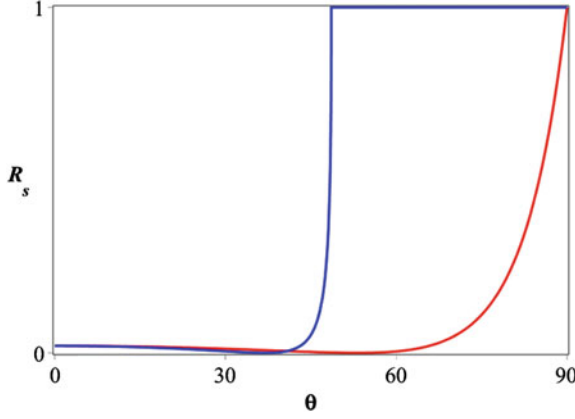
The reflectivity of the  $p$  polarization off a discontinuity in the dielectric function is shown in Fig. 1.4.

From (1.31) we see that the  $p$  wave shows zero reflection when  $Q_1 = Q_2$ , that is at the Brewster angle

$$\theta_B = \arctan \frac{n_2}{n_1}. \quad (1.33)$$

It is apparent from (1.24) that this angle has special significance not only for a sharp transition between two media, but for diffuse profiles as well. This is because the wave equation in the dilated variable  $Z$  links two media with effective wavevector components  $Q_1$ , and  $Q_2$  which are equal at this angle. The  $s$  and  $p$  effective wavevector components  $q$  and  $Q$  are shown in Fig. 1.5, which also illustrates the reason for small  $p$  reflectivity at the Brewster angle. The Figure shows  $q^2$  versus  $z$  and  $Q^2$  versus  $Z$  for the hyperbolic tangent profile

$$\varepsilon(z) = \frac{1}{2}(\varepsilon_1 + \varepsilon_2) - \frac{1}{2}(\varepsilon_1 - \varepsilon_2) \tanh \frac{z}{2a}, \quad (1.34)$$



**Fig. 1.4** Step profile reflectivity for the  $p$  wave, for the air-water interface. The curve for light incident from air is zero at the Brewster angle  $\arctan(4/3) \approx 53.1^\circ$ . For incidence from water the reflectivity is zero at the Brewster angle  $\arctan(3/4) \approx 36.9^\circ$ , and unity beyond the critical angle  $\theta_c = \arcsin(3/4) \approx 48.6^\circ$

for which the dilated  $z$  coordinate is

$$Z = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)z - (\varepsilon_1 - \varepsilon_2)a \ln \cosh\left(\frac{z}{2a}\right). \quad (1.35)$$

At the Brewster angle  $\theta_B$ ,

$$Q_1^2 = Q_2^2 = \frac{(\omega/c)^2}{\varepsilon_1 + \varepsilon_2} = Q_B^2, \quad (1.36)$$

$$K^2 = \varepsilon_1 \varepsilon_2 Q_B^2 = K_B^2 = \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \left(\frac{\omega}{c}\right)^2. \quad (1.37)$$

From (1.24), a general profile  $\varepsilon(z)$  has  $Q^2$  at the Brewster angle given by

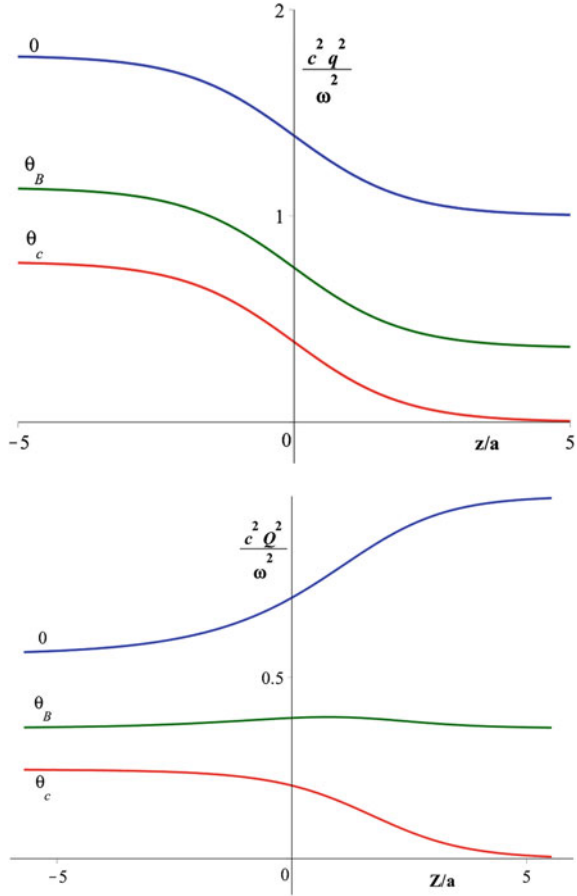
$$Q^2(\theta_B, z) = \frac{\frac{\omega^2}{c^2} \left\{ \varepsilon(z) - \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right\}}{\varepsilon^2(z)}. \quad (1.38)$$

Thus the bump in  $Q^2$  at the Brewster angle (see Fig. 1.5) has the analytic form

$$Q^2(\theta_B, z) - Q_B^2 = \frac{\omega^2}{c^2} \frac{(\varepsilon_1 - \varepsilon)(\varepsilon - \varepsilon_2)}{\varepsilon^2(\varepsilon_1 + \varepsilon_2)}. \quad (1.39)$$

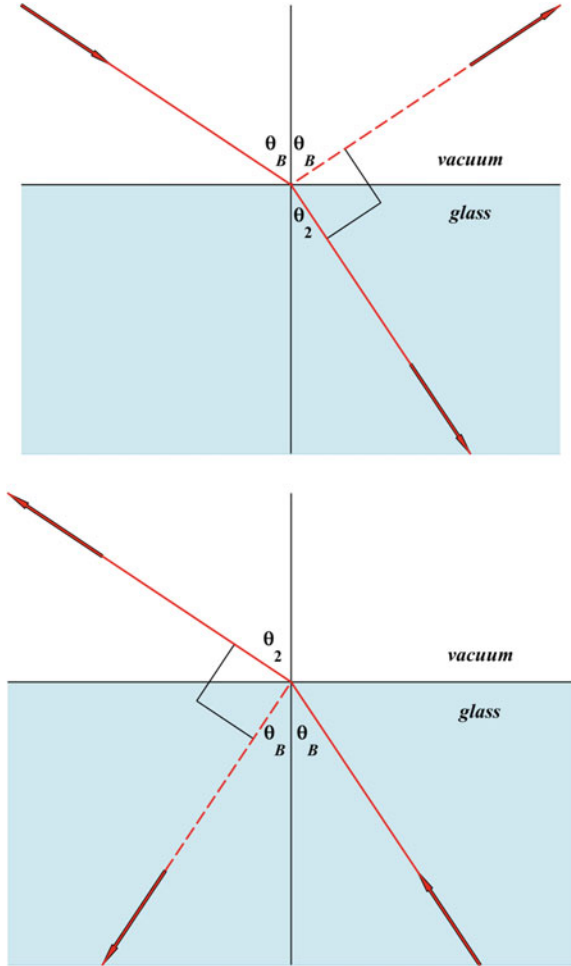
The  $p$  wave equation in the  $Z, Q$  notation has reflection at  $\theta_B$  due to the small variation in the effective wavevector component  $Q$  as given by (1.39). For the step profile,  $\varepsilon$  equals either  $\varepsilon_1$  or  $\varepsilon_2$ , and there is no variation in  $Q$  and thus no reflection.

**Fig. 1.5** Squares of the normal wavevector component  $q$  and of the effective normal component  $Q$  for the  $s$  and  $p$  waves. The figure shows  $q^2(z)$  and  $Q^2(Z)$  for the hyperbolic tangent dielectric function profile, at three angles of incidence. The *upper curve* (in each case) is for normal incidence, the *middle curve* is at the Brewster angle  $\theta_B = \arctan(n_2/n_1)$  and the *lower curve* is at the critical angle for total internal reflection,  $\theta_c = \arcsin(n_2/n_1)$ . The refractive indices  $n_1 = 4/3$  and  $n_2 = 1$  approximate the water/air interface. Water is on the *left* in both diagrams



A common explanation for the small reflection of the  $p$  polarization at  $\theta_B$  is in terms of the angular dependence of the dipole radiation from each atom or molecule which produces the transmitted and reflected waves. The far-field radiation pattern of a dipole has zero amplitude along the line of oscillation of the dipole (see Sect. 1.5, (1.78)). We see from (1.32) that  $r_{p0}$  is zero when  $\theta_1 + \theta_2 = \pi/2$ , that is when the refracted and reflected waves are at a right angle (see Fig. 1.6). The argument goes that at this angle of incidence there is no radiation from the accelerated electrons in the material to produce a  $p$ -polarized signal in the direction of specular reflection (upper part of Fig. 1.6). But zero reflection also exists in the reverse case of material to vacuum (lower figure). In this case the explanation in terms of electrons radiating along the transmitted beam to produce (or fail to produce) the reflected beam does not apply. Further, a similar case of zero reflection at the interface between two unlike media occurs with acoustic waves (as will be discussed in Sect. 1.4), and in that case the radiation from each scatterer does not have a dipole character.

**Fig. 1.6** Illustrating complete transmission of the  $p$  wave at the Brewster angle. In each case  $\theta_2 = \pi/2 - \theta_B$ , so the transmitted and non-reflected rays are at right angles



### 1.3 Particle Waves

In non-relativistic quantum mechanics, the motion of a particle of mass  $m$  and energy  $\mathcal{E}$  in a potential  $V$  is determined by Schrödinger's equation for the probability amplitude  $\Psi$ ,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = \mathcal{E}\Psi. \quad (1.40)$$

( $\hbar$  is Planck's constant divided by  $2\pi$ .) We shall consider reflection at a planar stratified boundary region between two uniform media characterized by potentials  $V_1$  and  $V_2$ . Examples of the particles and interfaces to which this description applies

are: electrons at a junction between two metals (with possibly an oxide layer in between); neutrons reflecting off a solid or liquid surface; and helium atoms reflecting at a liquid helium surface. In each of these examples the potential  $V$  in the single-particle equation (1.40) is an effective potential, representing the net effect of all the interactions between the particle and the scatterers in the medium through which it moves. An example of how this effective potential is determined is given in Sect. 1.5.

We again consider plane waves propagating in the  $zx$  plane, incident on a planar interface, with stratification in the  $z$  direction. For this geometry,  $V$  depends on one spatial variable  $z$ , and  $\Psi$  is independent of  $y$ . The  $z, x$  variable dependence in (1.40) is then separable, with

$$\Psi(z, x) = e^{iKx}\psi(z) \quad (1.41)$$

(it is usual to suppress the time dependence  $e^{-iEt/\hbar}$ ). Substitution of (1.41) into (1.40) gives an ordinary differential equation for  $\psi$ :

$$\frac{d^2\psi}{dz^2} + q^2\psi = 0, \quad q^2(z) = \frac{2m}{\hbar^2}[\mathcal{E} - V(z)] - K^2. \quad (1.42)$$

From (1.41),  $K$  is the  $x$ -component of the wavevector in either medium, and is an invariant of the motion, because of the absence of transverse components of the force,  $\partial V/\partial x = 0 = \partial V/\partial y$ . If the angles of incidence, reflection and refraction are  $\theta_1$ ,  $\theta'_1$ , and  $\theta_2$ , the laws of reflection and refraction follow from the invariance of  $K = k_{1x} = k'_{1x} = k_{2x}$ :

$$k_1 \sin \theta_1 = k_1 \sin \theta'_1 = k_2 \sin \theta_2, \quad (1.43)$$

where

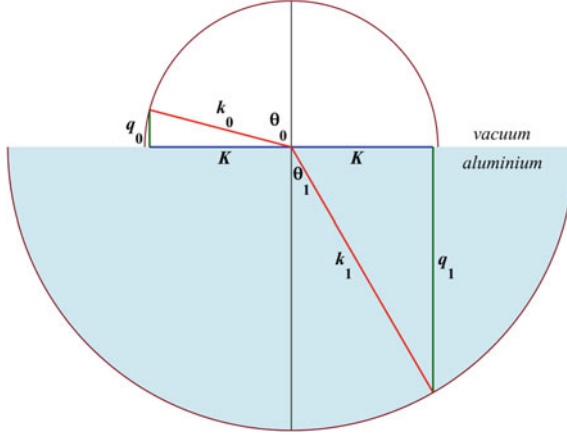
$$k_i^2 = K^2 + q_i^2 = \frac{2m}{\hbar^2}[\mathcal{E} - V_i]. \quad (1.44)$$

As before,  $q$  is the component of the wavevector normal to the interface, with limiting values

$$k_1 \cos \theta_1 = q_1 \leftarrow q(z) \rightarrow q_2 = k_2 \cos \theta_2. \quad (1.45)$$

These relations are summarized in Fig. 1.7.

On comparison of (1.7) and (1.42) we see that there is a one-to-one correspondence between the reflection problems for the electromagnetic  $s$  wave and particle waves obeying Schrödinger's equation, with the replacement



**Fig. 1.7** Graphical representation of  $k^2 = q^2 + K^2$  and of  $K = k_1 \sin \theta_1 = k_0 \sin \theta_0$ . (We use zero as subscript since in this example the upper medium is the vacuum;  $V_0$  is the vacuum potential, usually taken as zero.) The figure is drawn for electrons at 10 eV above the Fermi level in bulk aluminium, at the aluminium-vacuum interface.  $\mathcal{E}_F - V_1 \approx 11.7$  eV, so  $\mathcal{E} - V_1 \approx 21.7$  eV;  $V_0 - \mathcal{E}_F \approx 4.2$  eV, so  $\mathcal{E} - V_0 \approx 5.8$  eV; the ratio of the refractive indices is  $\{(\mathcal{E} - V_1)/(\mathcal{E} - V_0)\}^{1/2} \approx 1.934$

$$\varepsilon(z) \frac{\omega^2}{c^2} \leftrightarrow \frac{2m}{\hbar^2} [\mathcal{E} - V(z)]. \quad (1.46)$$

The reflection amplitude  $r$  and the transmission amplitude  $t$  are defined in terms of the limiting forms of the solution of (1.42):

$$e^{iq_1 z} + r e^{-iq_1 z} \leftarrow \psi(z) \rightarrow t e^{iq_2 z}. \quad (1.47)$$

For example, for the potential step

$$V_0(z) = \begin{cases} V_1 & (z < 0) \\ V_2 & (z > 0) \end{cases} \quad (1.48)$$

continuity of  $\psi$  and  $d\psi/dz$  at  $z = 0$  gives the Fresnel-type equations

$$r_0 = \frac{q_1 - q_2}{q_1 + q_2}, \quad t_0 = \frac{2q_1}{q_1 + q_2}. \quad (1.49)$$

Note that, as in the case of electromagnetic waves, the boundary conditions follow from the differential equations; they are not an additional assumption of the theory.

A refractive index can be defined for particles. From (1.43) and (1.44) we see that the refractive index is proportional to  $(\mathcal{E} - V)^{1/2}$ , that is to the square root of the kinetic energy, or to the local value of the wavevector  $k$ . The proportionality to

$(\mathcal{E} - V)^{1/2}$  is also a classical result: the equations for the conservation of energy and transverse momentum for a particle incident at angle  $\theta_1$  onto a planar stratification between media 1 and 2 read

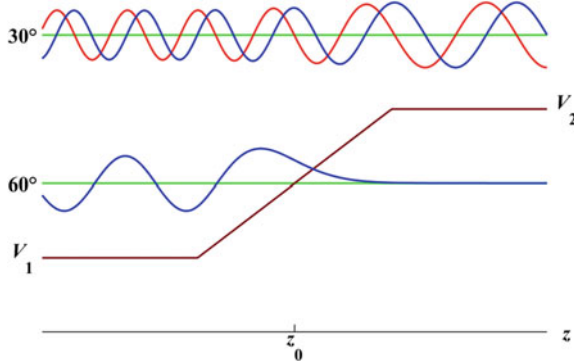
$$\frac{1}{2}mv_1^2 + V_1 = \mathcal{E} = \frac{1}{2}mv_2^2 + V_2, \quad (1.50)$$

$$mv_1 \sin \theta_1 = mv_2 \sin \theta_2. \quad (1.51)$$

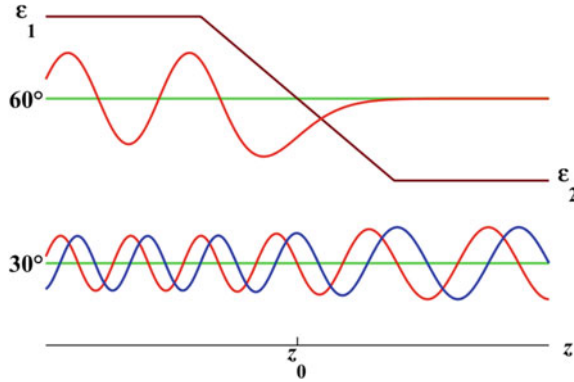
Equation (1.51) shows that the refractive indices are proportional to  $v_i$ , which from (1.50) are equal to  $[2(\mathcal{E} - V_i)/m]^{1/2}$ . However, partial reflection does not exist for classical particles: there is either total reflection (when  $V > \mathcal{E} - \frac{1}{2}m(v_1 \sin \theta_1)^2$  anywhere), or no reflection (when  $V < \mathcal{E} - \frac{1}{2}m(v_1 \sin \theta_1)^2$  everywhere).

In contrast, total reflection occurs in the wave theory only if  $V_2 > \mathcal{E} - \hbar^2 K^2/2m$ ;  $q_2$  is then imaginary, leading to exponential decay of the probability amplitude in medium 2. Regions of imaginary  $q$  (negative  $q^2 = (2m/\hbar^2)(\mathcal{E} - V) - K^2$ ) where  $V > \mathcal{E} - \hbar^2 K^2/2m$ , do not lead to *total* reflection when  $q_2$  is real, because of tunneling. Electromagnetic waves are likewise totally reflected when  $q_2$  is imaginary, that is when  $\varepsilon_2 \omega^2/c^2 < K^2$ , or  $\sin^2 \theta_1 > \varepsilon_2/\varepsilon_1$ . Thus the critical angle for total reflection is given by

$$\theta_c = \arcsin \left( \frac{\varepsilon_2}{\varepsilon_1} \right)^{1/2}, \quad \theta_c = \arcsin \left( \frac{\mathcal{E} - V_2}{\mathcal{E} - V_1} \right)^{1/2} \quad (1.52)$$



**Fig. 1.8** Probability amplitudes, at two angles of incidence, for particle waves incident from the left onto a linear ramp potential. The energy and potential values are such that  $\theta_c = 45^\circ$  ( $V_1:V_2:\mathcal{E} = 1:3:5$ ). The *upper two waves* are the real and imaginary parts of the probability amplitude  $\psi$  for incidence at  $30^\circ$ . The *lower curve* is the imaginary part of the probability amplitude for a totally reflected wave, incident at  $60^\circ$ . The real part is not shown, since the real and imaginary parts of  $\psi$  are proportional to each other in total reflection:  $\text{Im } \psi / \text{Re } \psi = \tan \delta/2$  when  $r = e^{i\delta}$  (Sect. 2.2). The classical turning point  $z_0$  (where  $q^2 = 0$ ) is halfway up the ramp



**Fig. 1.9** The electromagnetic  $s$  wave at two angles of incidence onto a linear dielectric function profile. The radiation is incident from the *left*. The dielectric constants are  $\epsilon_1 = 2, \epsilon_2 = 1$ , so that  $\theta_c = 45^\circ$ . The *lower two waves* are the real and imaginary parts of the electric field  $E(z)$ , at  $30^\circ$  angle of incidence. The *upper curve* is the real part of  $E(z)$  for a totally reflected wave incident at  $60^\circ$ . The curves are drawn at the level of  $(cK/\omega)^2$  for each angle of incidence. The wavefunctions for the electromagnetic  $s$  wave and for the particle waves of Fig. 1.8 are the same

in the electromagnetic and particle wave cases. Partial and total reflection of particle and electromagnetic  $s$  waves is compared in Figs. 1.8 and 1.9. Note that at  $30^\circ$  incidence the net flux at the right of the barrier,  $q_2|t|^2$ , is the same as the net flux on the left,  $q_1(1 - |r|^2)$ , despite the visible increase in the real and imaginary parts of the probability amplitude to the right. At  $60^\circ$  incidence the wave is totally reflected. The probability amplitudes are drawn about the levels  $\mathcal{E} - \hbar^2 K^2/2m$ , the energy available for motion in the  $z$  direction.

## 1.4 Acoustic Waves

There is an interesting close correspondence between the reflection of sound and the reflection of the electromagnetic  $p$  wave. This will be demonstrated in the simplest case of fluid, non-viscous media. Dissipation via viscosity and scattering can be accommodated by the use of a complex sound speed.

Sound waves propagate changes in density and pressure which are usually very small compared to the mean values. The equations of motion, continuity, and state can then be linearized by setting

$$\text{density} = \varrho + \varrho_a, \quad \text{pressure} = p + p_a, \quad (1.53)$$

where  $\varrho$  and  $p$  are the mean local values of the density and pressure, and  $\varrho_a$  and  $p_a$  are the small excess time-dependent values due to the presence of acoustic waves. On dropping second order terms in  $\varrho_a, p_a$  and in the velocity of a fluid element, and

neglecting the force due to gravity apart from its effect on stratification according to density, one obtains the equation (Bergmann 1946)

$$\nabla^2 p_a - \frac{1}{v^2} \frac{\partial^2 p_a}{\partial t^2} - \frac{1}{\varrho} \nabla \varrho \cdot \nabla p_a = 0. \quad (1.54)$$

Here  $v^2 = (\partial p / \partial \varrho)_s$  is the adiabatic derivative of the pressure with respect to density, and gives the square of the local phase velocity in the medium.

Consider now the reflection of sound at an interface characterized by a density profile  $\varrho(z)$  and an adiabatic pressure derivative  $(\partial p / \partial \varrho)_s = v^2(z)$ . For a plane monochromatic wave propagating in the  $zx$  plane, we have

$$p_a(z, x, t) = P(z) e^{i(Kx - \omega t)}. \quad (1.55)$$

$K$  is again the component of the wavevector along the interface, and is a constant of the motion:

$$K = \frac{\omega}{v_1} \sin \theta_1 = \frac{\omega}{v_2} \sin \theta_2, \quad (1.56)$$

where  $v_1, v_2$  are the limiting values of  $\{(\partial p / \partial \varrho)_s\}^{1/2}$  in the two media, and  $\theta_1, \theta_2$  are the angles of incidence and refraction. The differential equation for  $P$  is obtained by substitution of (1.55) into (1.54):

$$\varrho \frac{d}{dz} \left( \frac{1}{\varrho} \frac{dP}{dz} \right) + q^2 P = 0, \quad (1.57)$$

with

$$q^2(z) = \frac{\omega^2}{v^2(z)} - K^2; \quad (1.58)$$

$q$  is again the normal component of the wavevector, with limiting values  $q_1 = (\omega/v_1) \cos \theta_1, q_2 = (\omega/v_2) \cos \theta_2$ .

The term  $(d\varrho/dz)(dP/dz)$  in (1.57) may be removed by introducing a new dependent variable  $P/\sqrt{\varrho}$ , as Bergmann notes. This is analogous to the transformation to  $B/\sqrt{\varepsilon}$  discussed in Sect. 1.2. A more fruitful approach is analogous to the transformation to a dilated  $z$  variable in the  $p$  wave case: (1.57) has the same form as the electromagnetic  $p$  wave equation

$$\varepsilon \frac{d}{dz} \left( \frac{1}{\varepsilon} \frac{dB}{dz} \right) + q^2 B = 0$$

In terms of a new independent variable  $Z$ , defined by  $dZ = \varrho dz$ , (1.57) becomes

$$\frac{d^2 P}{dZ^2} + Q^2 P = 0, \quad Q = \frac{q}{\varrho}. \quad (1.59)$$

(As defined here,  $Z$  and  $Q$  no longer have the dimensions of length and of  $(\text{length})^{-1}$ ; this can be remedied by respectively dividing  $Z$  and multiplying  $Q$  by some density, for example  $(\varrho_1 + \varrho_2)/2$ .)

It is clear from the form of (1.59), and the discussion of reflection at the Brewster angle given in Sect. 1.2, that weak reflection of acoustic waves (zero reflection, in the case of a sharp transition between the two media) is expected whenever  $Q_1 = Q_2$ . This holds when

$$\frac{\cos \theta_1}{\varrho_1 v_1} = \frac{\cos \theta_2}{\varrho_2 v_2}. \quad (1.60)$$

This result was first given (for a sharp interface) by George Green (1838). On eliminating  $\theta_2$  from (1.60) and Snell's Law (1.56), one finds that weak reflection occurs at an angle of incidence  $\theta_1 = \theta_G$  (which we will call Green's angle) given by

$$\tan^2 \theta_G = \frac{(\varrho_2 v_2)^2 - (\varrho_1 v_1)^2}{\varrho_1^2 (v_1^2 - v_2^2)}. \quad (1.61)$$

In contrast to the electromagnetic  $p$  wave case, weak reflection of acoustic waves does not happen at a certain angle at a boundary between *any* two media: the quantities  $\varrho_1 v_1 - \varrho_2 v_2$  and  $v_1 - v_2$  must have opposite signs.

At Green's angle  $\theta_G$  (where  $Q_1 = Q_2$ ),  $K^2$  is equal to

$$K_G^2 = \frac{\omega^2}{\varrho_1^2 - \varrho_2^2} \left\{ \left( \frac{\varrho_1}{v_2} \right)^2 - \left( \frac{\varrho_2}{v_1} \right)^2 \right\}, \quad (1.62)$$

and the common value of  $Q_1$  and  $Q_2$  is given by

$$Q_G^2 = \frac{\omega^2}{\varrho_1^2 - \varrho_2^2} \left\{ \frac{1}{v_1^2} - \frac{1}{v_2^2} \right\}. \quad (1.63)$$

According to (1.59), the acoustic wave in the  $Z$  variable then reflects from the bump in  $Q^2$ , given by

$$Q^2 - Q_G^2 = \frac{\omega^2}{\varrho^2 (\varrho_1^2 - \varrho_2^2)} \left\{ \frac{\varrho_1^2 - \varrho_2^2}{v^2} - \left( \frac{\varrho_1}{v_2} \right)^2 + \left( \frac{\varrho_2}{v_1} \right)^2 - \varrho^2 \left( \frac{1}{v_1^2} - \frac{1}{v_2^2} \right) \right\}. \quad (1.64)$$

One can define an acoustic reflection amplitude  $r$  and a transmission amplitude  $t$  in terms of the pressure:

$$e^{iq_1 z} + r e^{iq_1 z} \leftarrow P(z) \rightarrow t e^{iq_2 z}. \quad (1.65)$$

For a sharp transition between media 1 and 2,  $P$  and  $dP/dz = dP/dZ$  are continuous at the boundary. (This is evident from (1.57); note that, as in the electromagnetic and particle wave cases, the differential equation dictates the boundary conditions, which are not an additional input to the theory.) Thus, for a sharp boundary located at the origin,

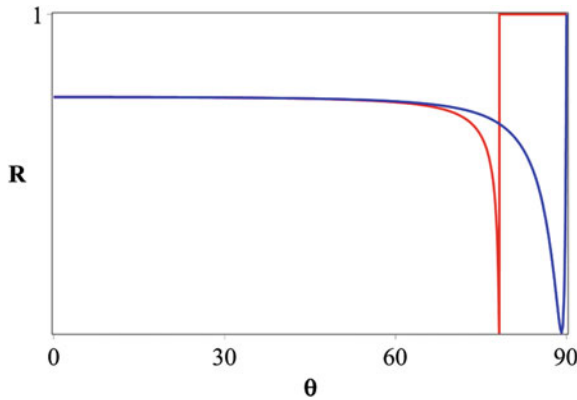
$$r = \frac{Q_1 - Q_2}{Q_1 + Q_2}, \quad t = \frac{2Q_1}{Q_1 + Q_2}. \quad (1.66)$$

These may be rewritten as

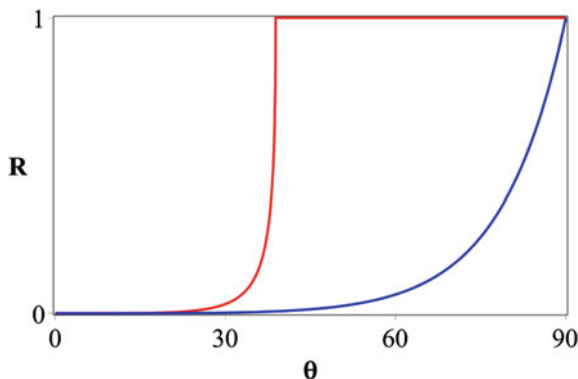
$$r = \frac{q_2 \tan \theta_2 - q_1 \tan \theta_1}{q_2 \tan \theta_2 + q_1 \tan \theta_1}, \quad t = \frac{2q_2 \tan \theta_2}{q_2 \tan \theta_2 + q_1 \tan \theta_1}. \quad (1.67)$$

Total reflection occurs for angles of incidence greater than

$$\theta_c = \arcsin\left(\frac{v_1}{v_2}\right). \quad (1.68)$$



**Fig. 1.10** Reflectivity of acoustic waves at a mercury-water interface, according to (1.66). For sound incident from the slower medium (mercury) total reflection occurs beyond the critical angle  $\theta_c \approx 78.21^\circ$ . Very close is the Green's angle  $\theta_G \approx 78.18^\circ$ , so the reflectivity changes from zero to unity in  $0.03^\circ$ . For sound incident from water the Green's angle is very close to glancing incidence,  $\theta_G \approx 89.12^\circ$ . Thus again the reflectivity changes from zero to unity very rapidly. The curves are drawn for  $\rho_{\text{Hg}}/\rho_{\text{H}_2\text{O}} = 13.57$ ,  $v_{\text{Hg}}/v_{\text{H}_2\text{O}} = 0.9789$



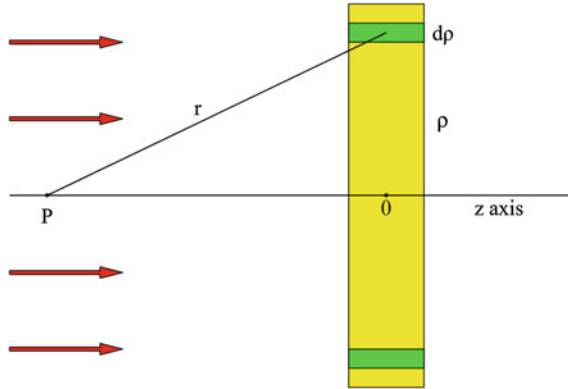
**Fig. 1.11** Reflectivity of acoustic waves at a water-carbon tetrachloride interface, obtained from (1.66). For sound incident from the slower medium ( $\text{CCl}_4$ ) the Green's angle is  $\theta_G \approx 1.73^\circ$ , and total reflection occurs beyond  $\theta_c \approx 38.86^\circ$ . For sound incident from water the Green's angle is  $\theta_G \approx 2.76^\circ$ . The curves are drawn for  $\rho_{\text{CCl}_4}/\rho_{\text{H}_2\text{O}} = 1.595$ ,  $v_{\text{CCl}_4}/v_{\text{H}_2\text{O}} = 0.6274$

This result follows on setting  $\theta_2 = \pi/2$  in (1.56); it holds for any interface, no matter how diffuse, provided absorption can be neglected. The critical angle  $\theta_c$  will be close to Green's angle  $\theta_G$ , if the latter exists, when  $v_1 \simeq v_2$ . The reflectivity of a step profile then rapidly goes from zero at  $\theta_G$  to unity at  $\theta_c$  and beyond, as illustrated for the mercury-water interface in Fig. 1.10.

When  $\varrho_1 v_1 \simeq \varrho_2 v_2$  the reflectivity at normal incidence is small, and  $\theta_G$  (if it exists) will also be small. This is the case for carbon tetrachloride and water, illustrated in Fig. 1.11.

## 1.5 Scattering and Reflection

Most of the results in this book come from analysis of the differential equations for waves in material media, the media being characterized by a dielectric function, or an effective potential, or the density and speed of sound, in the case of electromagnetic, particle or acoustic waves. This approach hides the many-body complexity of the real physics: specular reflection, for example, is the result of the constructive interference of many scattered or re-radiated waves. A discussion of reflection from this point of view will be given here; it leads to values for the functions characterizing the media, such as  $\varepsilon$  and  $V$ , in terms of the properties of the particles comprising the system. Such approaches go back to Lorentz (1909), Darwin (1924) and Hartree (1928) in the electromagnetic case. We will begin with an adaptation of Fermi's (1950) argument for the effective potential of a collection of neutron scatterers, since this is simpler.



**Fig. 1.12** Reflection of neutrons by a slab of scatterers. The thickness  $\Delta z$  of the slab is such that  $k\Delta z$  is small, so that the phase of the plane wave  $e^{ikz}$ , (incident from the left) is nearly constant over the slab

Consider the reflection of a *beam of neutrons* by a thin slab of material. The neutrons interact with the nuclei in the slab. For slow neutrons this interaction is characterized by a length  $b$ , the scattering length for neutrons off a bound scatterer. An incident plane wave  $e^{ikz}$  causes each scatterer to radiate a spherical wave  $-be^{ikr}/r$ . The reflected wave is found by summing up the scattered waves from all parts of the slab. The geometry is illustrated in Fig. 1.12.

If  $n$  is the number density of the scatterers,  $(2\pi\rho d\rho\Delta z)n$  is the number of scatterers within an annulus between  $\rho$  and  $\rho + d\rho$ , where  $\rho = \sqrt{x^2 + y^2}$  is the distance from the  $z$  axis. The reflected wave at  $P$  is thus

$$\psi_r = \int_0^\infty d\rho 2\pi\rho\Delta z n \left( -\frac{be^{ikr}}{r} \right). \quad (1.69)$$

For fixed  $z$  we have  $\rho d\rho = r dr$ , so that

$$\psi_r = -2\pi nb\Delta z \int_{-z}^\infty dr e^{ikr}. \quad (1.70)$$

The integral over  $r$  is not defined as it stands, because we have used  $e^{ikz}$  as the incident wave, namely a plane wave extending to infinity in the  $x$  and  $y$  directions. In practice the incident wave would be a finite beam, with an amplitude decreasing with  $\rho = (x^2 + y^2)^{1/2}$ . The resulting integral for  $\psi_r$  then is well-defined. When such

decrease is slow on the scale of  $k^{-1}$  (the beam is many wavelengths wide), the integral is equal to  $-e^{-ikz}/ik$ , and

$$\psi_r = \frac{2\pi n b \Delta z}{ik} e^{-ikz} \quad (1.71)$$

This is a reflected wave, with reflection amplitude equal to the coefficient of  $e^{-ikz}$ .

We will now show that the reflection amplitude due to a thin slab of thickness  $\Delta z$  and effective potential  $V$  is (to lowest order in  $V$ )

$$r_1 = \left( \frac{\Delta z}{2ik} \right) \frac{2mV}{\hbar^2}. \quad (1.72)$$

(What follows is heuristic; a rigorous proof is given in Chap. 3; see in particular (3.14).) Consider the effect of a potential hump, or well, which is small in extent in comparison with the wavelength. Seen on the scale of the wavelength, the hump appears as a spike, and its main effect is to create a change of slope in the wavefunction: on integrating (1.42) (at normal incidence) across the hump, we have

$$\psi'(z_2) - \psi'(z_1) = - \int_{z_1}^{z_2} dz \frac{2m}{\hbar^2} [\mathcal{E} - V(z)] \psi(z). \quad (1.73)$$

For wavelengths long compared to the extent of the hump,  $\psi$  is nearly constant over its effect, so when  $z_2 - z_1$  is small compared to  $k^{-1} = \hbar(2m\mathcal{E})^{-1/2}$ , and the hump is centred on the origin,

$$\psi'(z_2) - \psi'(z_1) \simeq \frac{2m}{\hbar^2} \psi(0) \int_{z_1}^{z_2} dz V(z) \quad (1.74)$$

(The zero of energy has been chosen so that  $V$  goes to zero on either side of the hump.) From (1.47) the left side is equal to  $ik(t - 1 + r) + O(k^2)$ . The assumption that  $\psi$  remains nearly constant from  $z_1$  to  $z_2$  also implies  $1 + r \simeq \psi(0) \simeq t$ . Thus (1.74) gives

$$r \simeq \left( \frac{1}{2ik} \right) \frac{2m}{\hbar^2} \int_{z_1}^{z_2} dz V(z). \quad (1.75)$$

For  $V$  constant inside the hump (of extent  $\Delta z$ ), and zero outside, this reduces to (1.72).

We can now give an expression for the effective potential of a collection of scatterers: (1.71) and (1.72) together imply that this is

$$V = 4\pi \left( \frac{\hbar^2}{2m} \right) nb. \quad (1.76)$$

The scattered waves interfere constructively to give a reflected and a transmitted wave, as if the medium were completely homogeneous and acted on the particles with a potential given by (1.76). We have considered normal incidence; at oblique incidence the constructive interference of the spherically diverging waves from the scatterers within the slab is in the specular and straight-through directions.

We now turn to the more complex question of *electromagnetic radiation* interacting with the atoms or molecules in a thin slab of material. We will calculate the field at  $P$  in front of a slab, as in Fig. 1.12. The incident electric field propagates in the  $z$  direction, and is taken to be polarized along the  $x$  direction,

$$\mathbf{E} = e^{i(kz - \omega t)} (E_0, 0, 0) \quad (1.77)$$

When the wavelength is large compared to atomic size, each atom radiates predominantly as a dipole. For a given atom with dipole  $\mathbf{p}$ , oscillating at the impressed angular frequency  $\omega$ , the electric field at  $\mathbf{r} = r\hat{\mathbf{r}}$  from the atom is (see for example Jackson (1975), Sect. 9.2)

$$\mathbf{E} = \frac{e^{ikr}}{r} \left\{ k^2 (\hat{\mathbf{r}} \times \mathbf{p}) \times \hat{\mathbf{r}} + [3(\hat{\mathbf{r}} \cdot \mathbf{p})\hat{\mathbf{r}} - \mathbf{p}] \left( \frac{1}{r^2} - \frac{ik}{r} \right) \right\}, \quad (1.78)$$

where  $k = \omega/c$ . The far field (given by the first term) is a spherically diverging wave, with  $\mathbf{E}$  transverse to  $\mathbf{r}$ . We do not omit the near field, since we do not wish to assume that  $kr \gg 1$ . All dipoles are taken to lie along the direction of the incident electric field, and to have the same strength  $\alpha E_0$ , where  $\alpha$  is the polarizability of an atom:

$$\mathbf{p} = e^{-i\omega t} (\alpha E_0, 0, 0) \quad (1.79)$$

The point  $P$  is at  $(0, 0, z)$ , with  $z < 0$ . The contribution to the electric field at  $P$  from a dipole at  $(x, y, 0)$  is then

$$E_x = \frac{\alpha E_0 e^{i(kr - \omega t)}}{r^3} \left\{ k^2 (y^2 + z^2) + (1 - ikr) \left( \frac{3x^2}{r^2} - 1 \right) \right\} \quad (1.80)$$

with  $E_y$  and  $E_z$  odd in  $x$  and thus integrating to zero when we sum over the dipolar fields. Thus the net field at  $P$  due to all the dipoles (of number density  $n$ ) in the thin slab is, on changing to the cylindrical coordinates  $\varrho$  and  $\phi$  and integrating over  $\phi$ ,

$$\begin{aligned}
E_x^{\text{dipoles}} &= e^{-i\omega t} \alpha E_0 n \pi \Delta z \int_0^\infty d\varrho \, \varrho \frac{e^{ikr}}{r^3} \left\{ k^2(\varrho^2 + 2z^2) + (1 - ikr) \left( \frac{3\varrho^2}{r^2} - 2 \right) \right\} \\
&= e^{-i\omega t} \alpha E_0 n \pi \Delta z \int_{-z}^\infty dr \frac{e^{ikr}}{r^2} \left\{ k^2(r^2 + z^2) + (1 - ikr) \left( 1 - \frac{3z^2}{r^2} \right) \right\}.
\end{aligned} \tag{1.81}$$

The first term is an integral of the form (1.70); the others may be obtained from it by integration by parts. The result is

$$E_x^{\text{dipoles}} = e^{-i(kz + \omega t)} 2\pi i k \alpha n \Delta z E_0. \tag{1.82}$$

The reflection amplitude for the slab is the coefficient of  $E_0 e^{-i(kz + \omega t)}$  in (1.82). We compare this with the result analogous to (1.72) for the reflection amplitude due to a thin slab of dielectric constant  $\varepsilon$ ,

$$r_1 = \frac{i}{2} k \Delta z (\varepsilon - 1). \tag{1.83}$$

Thus the effective dielectric constant of a slab of atoms of polarizability  $\alpha$  and number density  $n$  is

$$\varepsilon \simeq 1 + 4\pi\alpha n. \tag{1.84}$$

We have neglected the effects of the dipolar fields on each other. When these are taken into account, the resulting dielectric constant for a uniform medium becomes.

$$\varepsilon = \frac{1 + \frac{8}{3}\pi\alpha n}{1 - \frac{4}{3}\pi\alpha n}. \tag{1.85}$$

This expression is known as the Clausius-Mossotti or Lorentz-Lorenz formula (Lorentz 1909). The result (1.84) is the first-order term in the  $\alpha n$  expansion of (1.85). The form of (1.85), with  $n = n(z)$ , remains valid with a high degree of accuracy in a stratified medium of polarizable atoms (Castle and Lekner 1980; Lekner 1983).

## 1.6 A Look Ahead

In the preceding sections we have introduced the definitions and basic equations for the reflection of electromagnetic, particle and acoustic compressional waves by planar stratified media. The remainder of the book is written predominantly in

electromagnetic notation; a translation of the main results into particle-wave language is made in Chap. 15, and Chap. 16 deals with neutron and X-ray reflection. The final Chaps. 17–20 are on acoustic waves, chiral media, pulses and wavepackets, and finite beams. Here we preview the chapters, stating and discussing some of their results and techniques in order to give the reader a feel for the structure and content of the book.

Chapter 2 contains both general results, true for reflection and transmission at any transition between two homogeneous media, and some specific results for exactly solvable profiles. Among the general results are the conservation law

$$q_1(1 - |r_{12}|^2) = q_2|t_{12}|^2, \quad (1.86)$$

and reciprocity relations such as

$$r_{21} = -\frac{t_{12}}{t_{12}^*} r_{12}^* \quad (1.87)$$

and

$$q_2 t_{12} = q_1 t_{21}. \quad (1.88)$$

The conservation law (1.86), which holds for real  $q_1$  and  $q_2$  and in the absence of absorption within the interface, represents conservation of energy in the electromagnetic case, and conservation of probability density current in the particle case. The relation (1.87) holds under the same conditions, and implies that the reflectance  $R = |r|^2$  is the same from either side of incidence on a nonabsorbing interface. The relation (1.88) is more general, being valid also in the presence of absorption within the interface. It implies the equality of the transmittances  $T_{12} = (q_2/q_1)|t_{12}|^2$ ,  $T_{21} = (q_1/q_2)|t_{21}|^2$ , representing the energy or particle flux through the inhomogeneity, for incidence from medium 1 or from medium 2. (When the polarization subscripts  $s$  and  $p$  are omitted, the relation quoted is understood to be valid for either wave.)

For inhomogeneous interfaces extending from  $z_1$  to  $z_2$ , with  $\varepsilon = \varepsilon_1$  for  $z \leq z_1$  and  $\varepsilon = \varepsilon_2$ , the  $s$  wave reflection and transmission amplitudes may be expressed in terms of the values and derivatives of two linearly independent solutions  $F$  and  $G$  of (1.7) within  $z_1 \leq z \leq z_2$ , evaluated at  $z_1$  and  $z_2$ :

$$r_s = e^{2iq_1 z_1} \frac{q_1 q_2 (F_1 G_2 - G_1 F_2) + iq_1 (F_1 G'_2 - G_1 F'_2) + iq_2 (F'_1 G_2 - G'_1 F_2) - (F'_1 G'_2 - G'_1 F'_2)}{q_1 q_2 (F_1 G_2 - G_1 F_2) + iq_1 (F_1 G'_2 - G_1 F'_2) - iq_2 (F'_1 G_2 - G'_1 F_2) + (F'_1 G'_2 - G'_1 F'_2)}, \quad (1.89)$$

$$t_s = \frac{e^{i(q_1 z_1 - q_2 z_2)} 2iq_1 (F_2 G'_2 - G_2 F'_2)}{q_1 q_2 (F_1 G_2 - G_1 F_2) + iq_1 (F_1 G'_2 - G_1 F'_2) - iq_2 (F'_1 G_2 - G'_1 F_2) + (F'_1 G'_2 - G'_1 F'_2)}. \quad (1.90)$$

Similar expressions can be written down for the  $p$  polarization. These results are useful for specific profiles for which the solutions are known functions, such as the Airy functions for the linear profile, and the Bessel functions for the exponential profile. General results may also be deduced from (1.89) and (1.90), for example that  $r_s \rightarrow -1$  and  $t_s \rightarrow 0$  at grazing incidence, and that  $r_s$  and  $t_s$  tend to the Fresnel values (1.15) as  $\Delta z = z_2 - z_1$  tends to zero. From the  $p$  polarization expressions one finds that  $r_p \rightarrow 1$  and  $t_p \rightarrow 0$  at grazing incidence. Thus  $r_p/r_s$  always moves in the complex plane from  $+1$  at normal incidence to  $-1$  at grazing incidence, and the number of principal angles (or ellipsometric Brewster angles), defined by  $\text{Re}(r_p/r_s) = 0$ , is therefore always odd.

Chapter 2 also lists the exact solutions for three dielectric function profiles which are solvable for both the  $s$  and  $p$  polarizations, and another (the important hyperbolic tangent profile) which is solvable for the  $s$  wave only. Two other cases which are solvable for the  $s$  wave case, the  $\text{sech}^2(z/a)$  and the linear profile, are discussed in Sects. 4.3 and 5.2 respectively, where their solution is relevant to the problem at hand.

Chapter 3 treats the reflection of long waves, that is those whose wavelength is large compared to the thickness of the reflecting inhomogeneity. The long-wave results are obtained from perturbation theories, which in turn derive from exact integral and integro-differential equations obeyed by the  $s$  and  $p$  waves. For example, from the perturbation theory for the  $s$  wave one finds that the reflection amplitude, to second order in the interface thickness, is given by

$$r_s = r_{s0} + \frac{2q_1 \omega^2 / c^2}{(q_1 + q_2)^2} \left\{ i\lambda_1 - 2q_2 \lambda_2 - \frac{\omega^2 / c^2}{q_1 + q_2} \lambda_1^2 \right\} + \dots, \quad (1.91)$$

where the  $\lambda_n$  are integrals of dimension (length) <sup>$n$</sup> ,

$$\lambda_n = \int_{-\infty}^{\infty} dz [\varepsilon(z) - \varepsilon_0(z)] z^{n-1}. \quad (1.92)$$

In (1.92),  $\varepsilon(z)$  is the dielectric function profile under consideration, and  $\varepsilon_0(z)$  is the step dielectric function defined in (1.11), which has the reflection amplitude  $r_{s0}$  given in (1.13). The integrals  $\lambda_n$  depend on the relative positioning of the actual profile  $\varepsilon$  and the step profile  $\varepsilon_0$ . A theory which calculates reflection amplitudes as a perturbation series about a reference profile (here  $\varepsilon_0$ ) must obtain results for observables, such as  $|r_s|^2$ , which are invariant to the relative positioning of the actual and reference profile. If  $r = r_0 + r_1 + r_2 + \dots$ ,

$$R = |r|^2 = |r_0|^2 + 2 \operatorname{Re}(r_0^* r_1) + \{|r_1|^2 + 2 \operatorname{Re}(r_0^* r_2)\} + \cdots, \quad (1.93)$$

and we see from (1.91) that the first order term  $r_1$  is imaginary in the absence of absorption or total internal reflection for the  $s$  wave. (The same is true for the  $p$  wave, as is shown in Sect. 3.4.) Then there is no term in  $R$  of first order in the interface thickness, for either polarization. The second order term is given by the expression within the braces in (1.93); from (1.91) we have

$$R_1 = \left( \frac{q_1 - q_2}{q_1 + q_2} \right)^2 - \frac{4q_1 q_2 \omega^4 / c^4}{(q_1 + q_2)^4} i_2 + \cdots, \quad (1.94)$$

where the *integral invariant*  $i_2$  is given by

$$i_2 = 2(\varepsilon_1 - \varepsilon_2)\lambda_2 - \lambda_1^2. \quad (1.95)$$

(The subscript 2 denotes dimensionality (length)<sup>2</sup>.) The integrals  $\lambda_1$  and  $\lambda_2$  which enter into  $r_s$  and  $R_s$ , depend on the relative positioning of the actual and reference profiles, but the combination of integrals which comprise  $i_2$  is invariant with respect to the choice of positioning. Similar results are obtained for the observables  $r_p/r_s$ , and  $R_p = |r_p|^2$ :

$$\begin{aligned} r_{s0} \left( \frac{r_p}{r_s} \right) &= r_{p0} - \frac{2iQ_1}{(Q_1 + Q_2)^2} \frac{K^2}{\varepsilon_1 \varepsilon_2} I_1 + \cdots, \\ R_p &= \left( \frac{Q_1 - Q_2}{Q_1 + Q_2} \right)^2 \\ &- \frac{4Q_1 Q_2}{\varepsilon_1 \varepsilon_2 (Q_1 + Q_2)^4} \left\{ \frac{\omega^4}{c^4} i_2 - \frac{\omega^2}{c^2} K^2 \left[ j_2 + \left( \frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} \right) i_2 \right] + \frac{K^4}{\varepsilon_1 \varepsilon_2} [(\varepsilon_1 + \varepsilon_2) j_2 - I_1^2] \right\} + \cdots, \end{aligned} \quad (1.96)$$

In (1.97)  $j_2$  is another second order invariant, and the first order invariant  $I_1$  is defined by

$$I_1 = \int_{-\infty}^{\infty} dz \frac{(\varepsilon_1 - \varepsilon)(\varepsilon - \varepsilon_2)}{\varepsilon} = \int_{-\infty}^{\infty} dz \left\{ \varepsilon_1 + \varepsilon_2 - \frac{\varepsilon_1 \varepsilon_2}{\varepsilon} - \varepsilon \right\} \quad (1.98)$$

These results show that, in the long wave limit, the observables  $R_s$ ,  $R_p$ , and  $r_p/r_s$  take universal form. The integral invariants  $I_1$ ,  $i_1$ , and  $i_2$  depend on the profile shape and extent only. All frequency and angular dependence is contained in the coefficients of  $I_1$ ,  $i_1$ , and  $i_2$ , and is the same for all non-singular profiles. (The degenerate

case  $\varepsilon_1 = \varepsilon_2$  requires special consideration for the ellipsometric ratio  $r_p/r_s$  however.)

Equations (1.94), (1.96) and (1.97) illustrate how theory answers the question “what information can be obtained from a given experiment?” From (1.94) we see that measurement of the  $s$  reflectivity in the long wave case can determine only one characteristic of the interface, the invariant  $i_2$ . Experimental data at different angles of incidence give no new information (we are assuming that the interface has no roughness, and the absence of absorption in the interface or substrate), merely the opportunity to reduce the uncertainty in  $i_2$ . The same is true for ellipsometry to lowest order in the interface thickness: one parameter (the invariant  $I_1$ ) can be determined, at any angle of incidence. The  $p$  wave reflectance (1.97) carries more information, because the direction of the electric field relative to the interface changes with the angle of incidence. In principle, the values of  $I_1^2$ ,  $i_1$  and  $i_2$  may be determined by intensity measurements at a minimum of three angles of incidence.

The long wave results described above were obtained from perturbation theory, the perturbation being the deviation of the actual profile  $\varepsilon(z)$  from the step profile  $\varepsilon_0(z)$ . The simplest example of a perturbation theory expression for the reflection amplitude is that for reflection by a film between like media:

$$r_s^{\text{pert}} = -\frac{\omega^2/c^2}{2iq_0} \int_{-\infty}^{\infty} dz(\varepsilon - \varepsilon_0) e^{2iq_0 z}. \quad (1.99)$$

Here  $q_0$  is the common value of  $q_1$  and  $q_2$ ;  $\varepsilon_0$  is likewise the common value of  $\varepsilon_1$  and  $\varepsilon_2$ . The normal incidence, thin film version of this result has been used in Sect. 1.5 ((1.72) and (1.83)). Note that  $r_s^{\text{pert}}$  diverges at grazing incidence (as  $q_0 \rightarrow 0$ ). This is unphysical: for passive media the reflection amplitude must stay within the unit circle, and in fact we saw that the exact  $r_s$  tends to  $-1$  at grazing incidence.

This troublesome divergence at grazing incidence remains in higher order perturbation expressions, but is removed by the variational theory developed in Chap. 4. The simplest trial function,  $\psi_0 = e^{iq_0 z}$ , leads to the variational expression

$$r_s^{\text{var}} = \frac{-\frac{\omega^2/c^2}{2iq_0} \lambda(2q_0)}{1 + \frac{\omega^2/c^2}{2iq_0} \frac{\sigma(2q_0)}{\lambda(2q_0)}} \quad (1.100)$$

In this expression  $\lambda(2q_0)$  is the Fourier integral in (1.99), and  $\sigma(2q_0)$  is a double integral defined in Chap. 4. The variational result (1.100) is not divergent at grazing incidence; in fact it tends to the correct value of  $-1$  as  $q_0 \rightarrow 0$ , since the integrals  $\lambda$  and  $\sigma$  have the property that  $\sigma(0) = \lambda^2(0)$ . Further,  $r_s^{\text{var}}$  is correct to second order in the film thickness, whereas  $r_s^{\text{pert}}$  is not. These properties are shared by the variational expressions, derived in Chap. 4, for  $s$  and  $p$  wave reflection amplitudes between unlike media.

Non-linear, first order differential equations (of the Riccati type) for the reflection amplitudes are derived in Chap. 5. Two kinds of equations are used: those for a quantity  $q(z)$  which tends to  $re^{-2iq_1z}$  as  $z \rightarrow -\infty$ , and those for  $r(z)$ , tending to  $r$  in the same limit. For the  $s$  wave, the respective equations are

$$q' + 2iqq = \frac{q'}{2q} (1 - q^2), \quad (1.101)$$

$$r' = \frac{q'}{2q} (e^{2i\phi} - r^2 e^{-2i\phi}), \quad (1.102)$$

where primes denote differentiation with respect to  $z$ , and the phase integral  $\phi$  is defined by

$$\phi(z) = \int^z d\zeta q(\zeta). \quad (1.103)$$

The corresponding equations for the  $p$  wave reflection amplitudes have  $Q'/Q$  instead of  $q'/q$  on the right-hand side. From (1.101) it is shown in Sect. 5.4 that  $R_s$  has the Fresnel reflectivity as an upper bound for all monotonic profiles:

$$R_s \leq R_{s0} = \left( \frac{q_1 - q_2}{q_1 + q_2} \right)^2 \quad (1.104)$$

A similar bound holds for  $R_p$  when  $Q(z) = q(z)/\varepsilon(z)$  is monotonic.

Integration of (1.102) from  $z = -\infty$  to  $+\infty$  gives

$$r_s = - \int_{-\infty}^{\infty} dz \frac{q'}{2q} (e^{2i\phi} - r^2(z) e^{-2i\phi}). \quad (1.105)$$

The  $r(z)$  on the right-hand side is the reflection amplitude of a profile truncated at  $z$ . If the reflection is weak, one can get an approximate expression for  $r_s$  by omitting the term proportional to  $r^2$  on the right. This is the weak reflection or Rayleigh approximation,

$$r_s^R = - \int_{-\infty}^{\infty} dz \frac{q'}{2q} e^{2i\phi}. \quad (1.106)$$

The corresponding approximation in the  $p$  wave case is

$$r_p^R = \int_{-\infty}^{\infty} dz \frac{Q'}{2Q} e^{2i\phi}. \quad (1.107)$$

At normal incidence both (1.106) and (1.107) reduce to

$$r_n^R = -\frac{1}{2} \int_{-\infty}^{\infty} dz \frac{n'}{n} e^{2i\phi_n}, \quad \phi_n(z) = \frac{\omega}{c} \int^z d\zeta n(\zeta), \quad (1.108)$$

where  $n = \varepsilon^{1/2}$  is the refractive index. If one makes the further (and drastic) approximations of replacing  $2n$  by  $n_1 + n_2$  and  $\phi_n$  by  $(\omega/c)(n_1 + n_2)z = (k_1 + k_2)z$ , (1.108) simplifies to

$$r_n \simeq -\frac{1}{n_1 + n_2} \int_{-\infty}^{\infty} dz \frac{dn}{dz} e^{i(k_1 + k_2)z}. \quad (1.109)$$

Expressions closely related to (1.109) have been used by Buff et al. (1965) and by Huang and Webb (1969) in the analysis of reflection from the diffuse interface of a binary mixture.

The Rayleigh approximation works very well when the reflection is weak, but fails near grazing incidence. The Rayleigh approximation (1.106) and the long wave limiting form (1.94) are compared in Fig. 1.13 with the exact reflectivity for the hyperbolic tangent profile

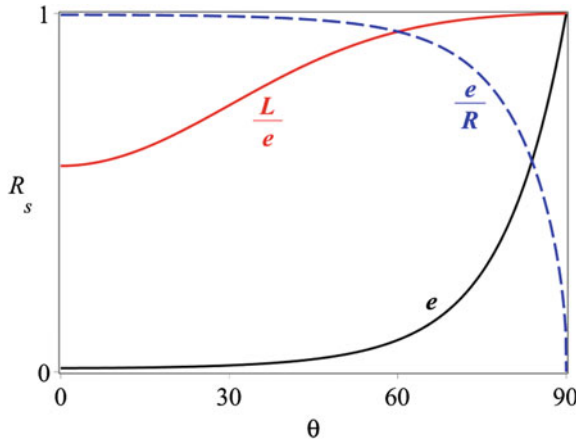
$$\varepsilon(z) = \frac{1}{2}(\varepsilon_1 + \varepsilon_2) - \frac{1}{2}(\varepsilon_1 - \varepsilon_2) \tanh \frac{z}{2a}. \quad (1.110)$$

For this profile the phase integral can be evaluated analytically (see Sect. 6.4),  $i_2 = (\pi^2/3)(\varepsilon_1 - \varepsilon_2)^2 a^2$  from Table 3.1, and the exact reflectivity is (from Sect. 2.5)

$$R_s = \left\{ \frac{\sinh \pi(q_1 - q_2)a}{\sinh \pi(q_1 + q_2)a} \right\}^2. \quad (1.111)$$

The figure illustrates the strengths and limitations of the long wave and weak reflection approximations: the long wave expression is good at glancing incidence, where the effective wavelength  $2\pi/q$  is large, while the Rayleigh approximation is good near normal incidence, but fails near glancing incidence, since the reflection is then strong (as always).

The reflection of short waves, that is those whose wavelength is small compared to the thickness of the interface, is discussed in Chap. 6. In the short wave limit the reflection properties usually approach the behaviour of classical particles, which are



**Fig. 1.13** Reflectivity of the  $s$  wave by the tanh profile (1.110), for  $\varepsilon_1 = 1$  and  $\varepsilon_2 = (4/3)^2$  and  $\omega a/c = 0.2$ . For this value of  $\omega a/c$  the distance in which the dielectric function changes over 80 % of its range (from  $(9\varepsilon_1 + \varepsilon_2)/10$  to  $(\varepsilon_1 + 9\varepsilon_2)/10$ ) is about one seventh of the wavelength of the incident radiation. The curve  $e$  is the exact reflectivity (1.111), the dashed curve  $e/R$  gives the ratio of the exact to the Rayleigh reflectivities, and the curve  $L/e$  gives the ratio of the long-wave limiting form (1.94) to the exact value

either totally reflected or not reflected. Away from classical turning points, which located at the zeros of  $q^2(z)$ , approximate solutions of (1.7) are the Liouville-Green functions

$$\psi_+ = \left(\frac{q_1}{q}\right)^{\frac{1}{2}} e^{i\phi}, \quad \psi_- = \left(\frac{q_2}{q}\right)^{\frac{1}{2}} e^{-i\phi} \quad (1.112)$$

( $\phi$  is the phase integral defined in (1.103)). A perturbation theory based on a Green's function constructed from  $\psi_{\pm}$  gives the first order reflection amplitude

$$r_s^{(1)} = -\frac{1}{2} \int_{-\infty}^{\infty} d\phi e^{2i\phi} \left\{ \gamma - \frac{\gamma^2}{4i} \right\}, \quad (1.113)$$

where

$$\gamma = \frac{1}{q^2} \frac{dq}{dz} = \frac{1}{q} \frac{dq}{d\phi} \quad (1.114)$$

is a dimensionless function which must be small for the short wave approximation to hold. The perturbation theory result is closely related to the Rayleigh approximation (which is the first term of another perturbation approach, the Bremmer series discussed in Sect. 6.5), as can be seen by writing (1.106) in the form

$$r_s^R = -\frac{1}{2} \int_{-\infty}^{\infty} d\phi \gamma e^{2i\phi}. \quad (1.115)$$

Unlike the long wave case, the reflection properties of short waves depend on the detail of the reflecting inhomogeneity, and do not take a universal form. For example: in the case of the profiles of finite range, which have a discontinuity in slope at the endpoints  $z_1$  and  $z_2$ , both  $r_s^{(1)}$  and  $r_s^R$  give

$$r_s = \frac{1}{4i} e^{i(\phi_1 + \phi_2)} \{ \gamma_1 e^{-i\Delta\phi} - \gamma_2 e^{i\Delta\phi} \} + \dots, \quad (1.116)$$

where  $\phi_1$  and  $\phi_2$  are the values of the phase integral at  $z_1$  and  $z_2$ ,  $\Delta\phi = \phi_2 - \phi_1$ , and  $\dots$  denotes that exponentially small terms have been omitted. (The function  $\gamma$  changes in value from 0 to  $\gamma_1$  at  $z_1$ , and from  $\gamma_2$  to 0 at  $z_2$ ). A similar result holds for the  $p$  wave:

$$r_p = \frac{1}{4i} e^{i(\phi_1 + \phi_2)} \{ \gamma_1 \cos 2\theta_1 e^{-i\Delta\phi} - \gamma_2 \cos 2\theta_2 e^{i\Delta\phi} \} + \dots. \quad (1.117)$$

Both the  $s$  and  $p$  reflectivities are thus oscillatory functions of  $\Delta\phi$ , and decay as the inverse square of the vacuum wavenumber  $\omega/c$ . The dominant part of the  $s$  reflectivity is

$$R_s = \frac{1}{16} \{ \gamma_1^2 + \gamma_2^2 - 2\gamma_1\gamma_2 \cos 2\Delta\phi \} + \dots. \quad (1.118)$$

(The  $p$  reflectivity has the same form, with  $\gamma \cos 2\theta$  replacing  $\gamma$ .) This oscillatory behaviour, with amplitude decreasing with frequency, is characteristic of profiles with discontinuities in slope or higher order derivatives. Profiles with no such discontinuities, such as the hyperbolic tangent, show exponential decrease with  $\omega a/c$  in the short wave limit,  $a$  being characteristic of the profile thickness.

Approximations such as (1.116) and (1.117), and the Rayleigh approximation, fail at grazing incidence, and in the presence of turning points. When there is a single turning point ( $q^2 \leq 0$  for  $z \geq z_0$ , say) there is total reflection. For the  $s$  wave

$$r_s = e^{i\delta_s}, \quad \delta_s \simeq 2 \int_0^{z_0} dz q(z) - \frac{\pi}{2}, \quad (1.119)$$

the phase decrement  $\pi/2$  being universal for smooth profiles. In the case of two turning points ( $q^2 < 0$  for  $z_1 \leq z \leq z_2$ ), the classically forbidden region  $q^2 < 0$  is tunneled through by a portion of the wave. The transmission amplitude then varies approximately as  $\exp(-2\Delta\Phi)$ , where  $\Delta\Phi$  is the increment in the imaginary part of the phase integral between the turning points:

$$\Delta\Phi = \int_{z_1}^{z_2} dz |q(z)|. \quad (1.120)$$

Reflection from anisotropic media is considered in Chaps. 7 and 8. Uniaxial systems are characterized by two dielectric functions  $\varepsilon_o(z, \omega)$  and  $\varepsilon_e(z, \omega)$ . The most general uniaxial reflection problem, with arbitrary orientation of the optic axis relative to the reflecting surface and the plane of incidence, is discussed in Chap. 8. In the simplest case where the system retains azimuthal symmetry about the normal to the interface (Chap. 7), the optic axis is also normal to the interface, and  $\varepsilon_o(z, \omega)$  and  $\varepsilon_e(z, \omega)$  give the response of the system to electric field components respectively parallel and perpendicular to the interface. The resolution of electromagnetic waves into  $s$  and  $p$  components remains valid in this case, with the equations to be satisfied modified from (1.7) and (1.20) to

$$\frac{d^2 E}{dz^2} + \left( \varepsilon_o \frac{\omega^2}{c^2} - K^2 \right) E = 0, \quad (1.121)$$

$$\frac{d}{dz} \left( \frac{1}{\varepsilon_o} \frac{dB}{dz} \right) + \left( \frac{\omega^2}{c^2} - \frac{K^2}{\varepsilon_e} \right) = 0. \quad (1.122)$$

Equation (1.121) has the same form as (1.7), with  $\varepsilon_o$  replacing  $\varepsilon$ , but (1.122) differs from the isotropic case, since it contains both  $\varepsilon_o$  and  $\varepsilon_e$ . There are corresponding changes in the  $p$  wave reflection amplitude, and in  $r_p/r_s$ . The ellipsometric ratio, for example, still takes the form (1.96) in the long wave case, but the invariant  $I_1$  is now given by

$$I_1 = \int_{-\infty}^{\infty} dz \left\{ \varepsilon_1 + \varepsilon_2 - \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_e} - \varepsilon_o \right\}. \quad (1.123)$$

(this applies to the case of an anisotropic thin film between isotropic media 1 and 2.) For reflection at a sharp boundary between an isotropic medium 1 and an anisotropic medium characterized by  $\varepsilon_o$  and  $\varepsilon_e$ , with its optic axis normal to the reflecting surface, there is zero reflection for the  $p$  polarization at

$$\theta_B = \arctan \left\{ \frac{\varepsilon_o(\varepsilon_o - \varepsilon_1)}{\varepsilon_1(\varepsilon_e - \varepsilon_1)} \right\}^{1/2}. \quad (1.124)$$

In the case of an anisotropic film, characterized by  $\varepsilon_o(z)$  and  $\varepsilon_e(z)$ , on a homogeneous anisotropic substrate characterized by  $\varepsilon_{2o}$  and  $\varepsilon_{2e}$ , the form (1.96) is still valid, with  $\varepsilon_{2e}$  replacing  $\varepsilon_2$  in the factor multiplying  $I_1$  and

$$I_1 = \int_{-\infty}^{\infty} dz \left\{ \frac{\varepsilon_1^2 - \varepsilon_{2o}\varepsilon_{2e}}{\varepsilon_1 - \varepsilon_{2o}} - \frac{\varepsilon_1 - \varepsilon_{2e}}{\varepsilon_1 - \varepsilon_{2o}} \varepsilon_o - \frac{\varepsilon_1 \varepsilon_{2e}}{\varepsilon_e} \right\}. \quad (1.125)$$

Ellipsometry is discussed in Chap. 9. The emphasis is on the analysis of what various ellipsometric configurations measure. We discuss transmission as well as reflection ellipsometry.

The effect of absorption (the dissipation of electromagnetic energy within the medium) is discussed in Chap. 10. Absorption is included phenomenologically in the Maxwell equations by means of a complex dielectric function,  $\varepsilon = \varepsilon_r + i\varepsilon_i$ . This simple change has far-reaching consequences for reflection properties. In the case of reflection at the sharp surface of an absorbing medium (a metal, for example), the Fresnel equations (1.13) and (1.31) retain their form, but now  $q_2 = q_r + iq_i$  and  $Q_2 = Q_r + iQ_i = (q_r + iq_i)/(\varepsilon_r + i\varepsilon_i)$ , where

$$\left(\frac{cq_r}{\omega}\right)^2 = \frac{1}{2} \left\{ \varepsilon_r - \varepsilon_1 \sin^2 \theta_1 + [(\varepsilon_r - \varepsilon_1 \sin^2 \theta_1)^2 + \varepsilon_i^2]^{\frac{1}{2}} \right\}, \quad (1.126)$$

$$\frac{cq_i}{\omega} = \frac{\varepsilon_i/2}{cq_i/\omega}. \quad (1.127)$$

The ellipsometric ratio  $r_p/r_s$  no longer has the real axis as its trajectory, but lies within the upper half of the unit circle:

$$\frac{r_p}{r_s} = \frac{q_1^2(q_r^2 + q_i^2) - K^4 + 2iq_1q_iK^2}{(q_1q_r + K^2)^2 + q_1^2q_i^2}. \quad (1.128)$$

Some of the general results derived in Chap. 2 still hold, notably the fact that  $r_s \rightarrow -1$  and  $r_p \rightarrow 1$  at grazing incidence, and the implication that there is an odd number of principal angles of incidence at which  $\text{Re}(r_p/r_s) = 0$ . The reciprocity relation (1.88) also holds, and thus the transmittance of an absorbing system is independent of the direction of propagation of the radiation.

Zero reflection is not possible off an absorbing medium with a sharp boundary, for either polarization. If however a dielectric layer is deposited on the absorber, zero reflectance is possible for both polarizations (at different angles of incidence); this interference-absorption effect thus produces reflection polarizers (Sect. 10.3).

A thin absorbing film on a transparent substrate always decreases the transmittance, but reflectance can be either increased or decreased, depending on the polarization and whether  $\varepsilon_1 < \varepsilon_2$  or  $\varepsilon_1 > \varepsilon_2$ . For example, the  $s$  reflectivity to first order in the film thickness is given by

$$R_s = \left(\frac{q_1 - q_2}{q_1 + q_2}\right)^2 - \frac{4q_1(q_1 - q_2)}{(q_1 + q_2)^3} \frac{\omega^2}{c^2} \int_{-\infty}^{\infty} dz \varepsilon_i(z) + \dots \quad (1.129)$$

The form (1.96) for the ellipsometric ratio is still valid, with  $I_1$  complex:

$$I_1 = \int_{-\infty}^{\infty} dz \left( \varepsilon_1 + \varepsilon_2 - \frac{\varepsilon_1 \varepsilon_2 \varepsilon_r}{\varepsilon_r^2 + \varepsilon_i^2} - \varepsilon_r \right) + i \int_{-\infty}^{\infty} dz \left[ \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_r^2 + \varepsilon_i^2} \right] \varepsilon_i. \quad (1.130)$$

An important and dramatic effect due to absorption is that of *attenuated total reflection*, discussed in Sect. 10.6. An absorbing layer (typically a metal film) deposited between two dielectrics can turn a total reflection configuration into one whose  $p$  reflectance is small at resonance, and can be zero for proper choice of thickness of metal film and angle of incidence. This phenomenon is an interference-attenuation effect, associated with the resonant excitation of electromagnetic surface waves at a metal-dielectric interface.

Chapter 11 deals with the inversion of reflectance and ellipsometric data to obtain the parameters of the reflector. For example, if the real and imaginary parts  $q_r$  and  $q_i$  of  $r_p/r_s$  are measured at angle of incidence  $\theta_1$  and the interface is known to be sharply defined on the scale of the wavelength, the real and imaginary parts of  $\varepsilon$  may be found from

$$\frac{\varepsilon_r + i\varepsilon_i}{\varepsilon_1} = \sin^2 \theta_1 + \sin^2 \theta_1 \tan^2 \theta_1 \frac{(1 - q_r^2)^2 - 4q_i^2 + 4i(1 - q_r^2)q_i}{[(1 - q_r)^2 + q_i^2]^2}. \quad (1.131)$$

If a model reflection amplitude is constructed as a function of wave vector component in medium 1, and analytically continued to negative  $q_1$  via  $r(-q_1) = r^*(q_1)$ , an explicit inversion is possible (Sect. 11.3) to obtain the dielectric function profile which would give this reflection amplitude in the Rayleigh approximation. In the  $s$  wave case the result is

$$\frac{\varepsilon(x)}{\varepsilon_1} \simeq \sin^2 \theta_1 + \cos^2 \theta_1 \exp \left( -4 \int_{-\infty}^{2x} dy F_s(y) \right), \quad (1.132)$$

where  $x = q_1^{-1} \int^z d\zeta q(\zeta)$  and  $F_s$  is the Fourier transform of  $r_s$ :

$$F_s(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dq_1 e^{-iq_1 y} r_s(q_1). \quad (1.133)$$

Matrix and numerical methods are developed in Chap. 12. Any stratified medium may be approximated by a set of homogeneous layers. The matrix methods connect, via a two-by-two matrix, the coefficients of either the two independent solutions, or the field amplitude and its derivative, at the entry and exit points of a layer. In the latter case these matrix relations for a homogeneous layer between  $z_n$  and  $z_{n+1}$  are as follows: for the  $s$  wave, with  $D = dE/dz$ ,

$$\begin{pmatrix} E_{n+1} \\ D_{n+1} \end{pmatrix} = \begin{pmatrix} \cos \delta_n & q_n^{-1} \sin \delta_n \\ -q_n \sin \delta_n & \cos \delta_n \end{pmatrix} \begin{pmatrix} E_n \\ D_n \end{pmatrix}. \quad (1.134)$$

For the  $p$  wave, with  $C = \varepsilon^{-1} dB/dz$ ,  $Q_n = q_n/\varepsilon_n$ , the matrix relation is

$$\begin{pmatrix} B_{n+1} \\ C_{n+1} \end{pmatrix} = \begin{pmatrix} \cos \delta_n & Q_n^{-1} \sin \delta_n \\ -Q_n \sin \delta_n & \cos \delta_n \end{pmatrix} \begin{pmatrix} B_n \\ C_n \end{pmatrix}. \quad (1.135)$$

For a profile approximated by  $N$  homogeneous layers, the reflection and transmission properties are determined by the profile matrix, which is a product of  $N$  layer matrices such as those in (1.134) or (1.135). If the elements of the profile matrix for the  $s$  polarization are  $s_{ij}$ , for example, the reflection and transmission amplitudes for an interface between media  $a$  and  $b$  are

$$r_s = e^{2i\alpha} \frac{q_a q_b s_{12} + s_{21} + i q_a s_{22} - i q_b s_{11}}{q_a q_b s_{12} - s_{21} + i q_a s_{22} + i q_b s_{11}}, \quad (1.136)$$

$$t_s = e^{i(\alpha-\beta)} \frac{2i q_a}{q_a q_b s_{12} - s_{21} + i q_a s_{22} + i q_b s_{11}}. \quad (1.137)$$

(Here  $\alpha = q_a z_1$  and  $\beta = q_b z_{N+1}$ ,  $z_1$  and  $z_{N+1}$  being the boundaries of the inhomogeneity.) In the absence of absorption the matrix elements are real. The matrix formulation, and the results (1.136) and (1.137), remain valid in the presence of absorption also, but the matrix elements are now complex.

The matrices in (1.134) and (1.135) are unimodular (have unit determinant); this fact simplifies the treatment of *periodically stratified media* (Sect. 12.3 and Chap. 13), which in turn has important application to the multilayer dielectric mirrors. Numerical methods based on the matrix formulation are also discussed in Chap. 12. Reflection of  $s$  waves by an arbitrary layer extending from  $a$  to  $b$  can be represented, to second order in the layer thickness, by the  $s$  matrix

$$\begin{pmatrix} 1 - \int_a^b dz q^2(z)(b-z) & b-a \\ -\int_a^b dz q^2(z) & 1 - \int_a^b dz q^2(z)(z-a) \end{pmatrix}. \quad (1.138)$$

(This result, and a similar one for the  $p$  matrix, are derived in Sect. 12.4.) In Sect. 12.8, a given interface is approximated by a set of layers within which the dielectric function  $\varepsilon(z)$ , and thus also  $q^2(z)$ , vary linearly with  $z$ . The matrix methods can be applied without modification to total reflection and tunneling; reflection and transmission through absorbing layers requires computation with complex matrix elements, the formalism being otherwise unaltered. Wavefunctions within the stratification may be obtained as a by-product of the profile matrix calculation.

Chapter 14 deals with reflection from rough surfaces. A planar stratified surface, no matter how diffuse, gives specular reflection of an incident plane wave, but rough surfaces scatter as well as reflect. The Rayleigh criterion for negligible roughness is (Sect. 14.1)

$$qh \ll 1 \quad (1.139)$$

where  $q$  (as always) is the normal component of the wavevector, and  $h$  is a measure of the variation in the height of the surface. When (1.139) is satisfied the surface will reflect specularly. According to the Rayleigh criterion, for given roughness and angle of incidence long waves may be reflected specularly and short waves diffusely, or for given roughness and wavelength there may be diffuse scattering near normal incidence and specular reflection near grazing incidence. Chapter 14 treats the reflection from corrugated surfaces (diffraction gratings), from liquid metal and liquid dielectric surfaces (scattering by thermally excited surface waves), in both cases using the methods of Rayleigh, and gives an outline of the application of the Helmholtz theorem to the scattering by rough surfaces (the Kirchhoff or surface integral method).

Chapter 15 adapts the content of the previous chapters to the language of particle waves obeying the Schrödinger equation. There follow three new chapters on special topics: 16 *Neutron and X-ray reflection*, 17 *Acoustic waves*, and 18 *Chiral isotropic media*.

In the last two chapters we finally move away from the assumption that the incident field consists of unbounded plane waves: the reflection of electromagnetic pulses and particle wavepackets is considered in Chap. 19, and that of finite beams in Chap. 20. We find that nearly monochromatic pulses reflect (in the first approximation) without change of shape, with a time delay  $\Delta t$  determined by the frequency variation of the phase of the reflection amplitude:

$$\Delta t = \frac{d\delta}{d\omega}. \quad (1.140)$$

(The derivative is to be evaluated at the dominant angular frequency of the pulse.) For example: total reflection at normal incidence has  $r_n = e^{i\delta_n}$ , and the short wave limiting form is found from (1.119) to be

$$\delta_n = 2\frac{\omega}{c} \int_0^{z_0} dz n(z, \omega) - \frac{\pi}{2}, \quad (1.141)$$

where  $n(z, \omega)$  is the refractive index, and  $z_0$  is the turning point determined by  $n(z_0, \omega) = 0$ . (This formula applies to reflection from the ionosphere, for example, in which case  $n^2 = \varepsilon \simeq 1 - \omega_p^2/\omega^2$ , where  $\omega_p$  is the plasma angular frequency, proportional to the square root of ionospheric electron density.) From (1.140) and

(1.141) we find that the time delay is the same as for pulse travel to the turning point and back at the group velocity  $u(z, \omega) = d\omega/dk$ , where  $k = n\omega/c$ :

$$\Delta t = 2 \int_0^z \frac{dz}{u} = \frac{2}{c} \int_0^{z_0} dz \left[ n + \omega \frac{\partial n}{\partial \omega} \right]. \quad (1.142)$$

The Appendix of Chap. 19 summarises the universal properties of electromagnetic pulses. The other parts of Chap. 19 deal with the reflection of particle wavepackets, illustrated by exact solutions.

Pulses are built up from waves of differing frequencies. Bounded beams (Chap. 20) can be regarded as superpositions of plane waves of differing directions of propagation. Just as the reflection of pulses is determined by the frequency dependence of the reflection amplitude, the reflection of beams depends on the angular dependence of the reflection amplitude. There is a lateral shift on reflection of a beam of radiation,

$$\Delta x = -\frac{d\delta}{dK}, \quad (1.143)$$

where  $K$  is the lateral component of the wavevector ( $K = k_x$ ), and the derivative is to be evaluated at the dominant value of  $K$  for the incident beam. A particularly interesting case is total reflection at a sharp boundary. For  $\theta_1 > \theta_c$  the phase of the  $s$  wave reflection amplitude is

$$\delta_s = -2 \arctan \frac{|q_2|}{q_1}, \quad (1.144)$$

and (1.143) leads to the beam shift

$$\Delta x_s = \frac{2K}{q_1|q_2|} = \frac{\lambda_1}{\pi} \frac{\tan \theta_1}{(\sin^2 \theta_1 - \sin^2 \theta_c)^{1/2}}, \quad (1.145)$$

where  $\lambda_1$  is the wavelength  $2\pi/k_1 = 2\pi c/n_1\omega$  in the first medium. This beam shift is divergent at the critical angle (where  $q_2 = 0$ ), and in fact the formula (1.139) fails there, since (1.143) is derived on the assumption of a slow variation of the phase shift with angle. In practice (1.145) works well to close proximity of the critical angle, as discussed in Sect. 20.2. Appendix 1 in Chap. 20 we show that the  $|q_2|$  singularity in the phase shift at  $\theta_1 = \theta_c^+$  is universal for nonabsorbing profiles. Finally, Appendix 2 in Chap. 20 outlines the somewhat surprising polarization properties of finite electromagnetic beams.

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## Further Readings

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*A detailed discussion of all aspects of ellipsometry can be found in Chapter 9 and in Azzam RMA, Bashara NM (1977) Ellipsometry and polarized light. See also Muller RH (1972) "Principles of ellipsometry", Advances in Electrochemistry and Electrochemical Engineering, vol. 9, Interscience*

*Sections 1.1 and 1.3 are based in part on*

Lekner J (1982a) Reflection of long waves by interfaces. *Physica* 112A:544–556

*The polarization of light by reflection from glass at  $56^\circ$  incidence, and from water at  $53^\circ$ , was discovered by Malus in 1808. In 1814 Brewster found, as the result of extensive experiments, that "the Index of refraction is the tangent of the angle of polarization". See*

Brewster D (1853) *A treatise on optics*, Longman, Brown and Green (Chapter 24)

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*The explanation of near transparency of a general interface to the p wave given in Section 1.2, and of the similar effect in the reflection of acoustic waves (Section 1.4), is based on*

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*For a treatment of the molecular basis of reflection see*

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Theory of Reflection

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