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SECOND-ORDER ELLIPSOMETRIC COEFFICIENTS

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We derive analytic expressions for the reflection amplitudes of s and p polarized electromagnetic radiation incident on a planar interface profile of arbitrary form, to second order in the parameter qa, where q is the component of the wavenumber perpendicular to the interface, and a is a length proportional to the interface thickness. New comparison identities, relating the reflection and transmission amplitudes of the p-wave to those for any reference profile, are derived. The second-order results are obtained by using one of these identities, and an integro-differential form of the p-wave equation.

1. Introduction

In a recent paper[1]) we considered waves satisfying the equation

$$\frac{d^2\psi}{dz^2} + q^2(z)\psi = 0 \tag{1}$$

and incident from medium 1, i.e. with the boundary condition

$$e^{iq_1z} + r\,e^{-iq_1z} \leftarrow \psi(z) \rightarrow t\,e^{iq_2z}. \tag{2}$$

We showed that the reflection amplitude r, and the transmission amplitude t, are given by

$$r = \frac{q_1 - q_2}{q_1 + q_2}\{1 - 2q_1q_2l^2\} + \mathcal{O}(qa)^3, \tag{3}$$

$$t = \frac{2q_1}{q_1 + q_2}\{1 + \tfrac{1}{2}(q_1 - q_2)^2l^2\} + \mathcal{O}(qa)^3. \tag{4}$$

Thus, as may be expected, the reflection and transmission amplitudes in the long wavelength limit are given by the amplitudes for a step profile (in which the transition from medium 1 to medium 2 is discontinuous), plus a correction term dependent on the deviation of the actual profile from a step profile. This is seen explicitly in the expression for the length l:

$$l^2 = 2 \int_{-\infty}^{\infty} \mathrm{d}z\, z(q^2 - q_{\mathrm{step}}^2)/(q_1^2 - q_2^2). \tag{5}$$

The reference step profile is positioned so as to make

$$\int_{-\infty}^{\infty} \mathrm{d}z(q^2 - q_{\mathrm{step}}^2) = 0 \tag{6}$$

(see fig. I-1). This positioning makes l invariant with respect to the choice of origin. The magnitudes $|r|$ and $|t|$ are thus also independent of the choice of origin, but the absolute phases are not. Here, as in I, we shall take the origin at the step, which is positioned to satisfy (6).

We saw in I that the above results are immediately applicable to the electromagnetic s-wave, in which the electric field is perpendicular to the plane of incidence. When the interface lies in the xy plane, and the propagation is in the zx plane, $\boldsymbol{E} = (0, E_y, 0)$, and E_y satisfies[2])

$$\nabla^2 E_y + \epsilon \frac{\omega^2}{c^2} E_y = 0 \tag{7}$$

(c is the speed of light, and ω is the angular frequency of the (monochromatic) wave). The dielectric function ϵ is primarily a function of z, but there is some x, y dependence. Part of the x, y dependence exists for the same reason that ϵ is not constant in the bulk phase: there are fluctuations in density, molecular orientation, or composition. In addition, there are surface contributions, arising out of surface roughness, or fluctuations in surface properties such as adsorption. In this paper we shall neglect the x, y dependence; this amounts to calculating reflections from an averaged sample. We also neglect anisotropy in the dielectric function (which has been shown to exist even in the solid–vapour[3]) and liquid–vapour[4]) interfaces of a monatomic system, but is there small). With these assumptions, $\epsilon = \epsilon(z)$, and the solution of (7) is in the form $E_y = \mathrm{e}^{\mathrm{i}Kx} E(z)$, where $E(z)$ satisfies

$$\frac{\mathrm{d}^2 E}{\mathrm{d}z^2} + \left(\epsilon \frac{\omega^2}{c^2} - K^2\right) E = 0. \tag{8}$$

K is the x-component of the wavevector in either medium, so if θ_1 and θ_2 are the angles of incidence and refraction, $K = k_1 \sin\theta_1 = k_2 \sin\theta_2$, where $k_i = \sqrt{\epsilon_i}\, \omega/c$. Eq. (8) is of the form (1), with

$$q^2(z) = \epsilon(z) \frac{\omega^2}{c^2} - K^2. \tag{9}$$

Thus q is the normal component of the wavenumber, and has the limiting forms

$$q_1 = k_1 \cos\theta_1 \leftarrow q(z) \rightarrow q_2 = k_2 \cos\theta_2. \tag{10}$$

For the s-wave we thus have from (3), (5) and (9) that

$$r_s = \frac{q_1 - q_2}{q_1 + q_2}\left\{1 - 4q_1q_2 \int_{-\infty}^{\infty} dz\, z\, \frac{\epsilon - \epsilon_{\text{step}}}{\epsilon_1 - \epsilon_2}\right\} + \mathcal{O}(qa)^3. \tag{11}$$

Thus the deviation from the step reflection amplitude in the long wavelength limit is expected to be of the form

$$\frac{r - r_{\text{step}}}{r_{\text{step}}} = -2k_1k_2l^2 \cos\theta_1 \cos\theta_2 + \mathcal{O}(qa)^3, \tag{12}$$

and to give information about one length l, where

$$(\epsilon_1 - \epsilon_2)l^2 = 2\int_{-\infty}^{\infty} dz\, z(\epsilon - \epsilon_{\text{step}}) = -\int_{-\infty}^{\infty} dz\, z^2 \frac{d\epsilon}{dz} \tag{13}$$

(subject to $\int_{-\infty}^{\infty} dz(\epsilon - \epsilon_{\text{step}}) = 0$). Values of l are given for five profiles in I; l^2 is positive for montonic profiles, which as expected reflect less than a step linking the same ϵ_1, ϵ_2.

The remainder of this paper will be concerned with calculating the reflection amplitude for the p-wave, in which the $\boldsymbol{B}$ vector is perpendicular to the plane of incidence. Thus, in our geometry, $\boldsymbol{B} = (0, B_y, 0)$. We will consider non-magnetic materials only, and assume that $\epsilon = \epsilon(z)$ as before. Then $B_y = e^{iKx}B(z)$, where $B(z)$ satisfies[2])

$$\frac{d^2B}{dz^2} - \frac{1}{\epsilon}\frac{d\epsilon}{dz}\frac{dB}{dz} + \left(\epsilon\frac{\omega^2}{c^2} - K^2\right)B = 0, \tag{14}$$

with

$$e^{iq_1z} - r_p\, e^{-iq_1z} \leftarrow B(z) \rightarrow \sqrt{\frac{\epsilon_2}{\epsilon_1}}\, t_p\, e^{iq_2z}. \tag{15}$$

The reason for the factors -1 and $\sqrt{\epsilon_2/\epsilon_1}$ multiplying r_p and t_p is that we wish r_s and r_p, and t_s and t_p, to refer to the same quantity, here chosen to be the electric field. The above factors follow from $\boldsymbol{E} = (ic/\epsilon\omega)\nabla \times \boldsymbol{B}$, the time-harmonic consequence of $\nabla \times \boldsymbol{B} = (\epsilon/c)\partial \boldsymbol{E}/\partial t$.

2. Near-transparency at the Brewster angle

We showed in section 5 of I that the p-wave equation (11) may be transformed to

$$\frac{d^2B}{dZ^2} + Q^2B = 0, \tag{16}$$

where $Q = q/\epsilon$ and the new variable Z is defined by

$$dZ = \epsilon\, dz, \quad Z = \int_0^z dz\epsilon(z). \tag{17}$$

In terms of the dilated new z-variable, the B equation is as simple as the E equation, but we now have Z depending on the shape of the dielectric profile. We will find the Z, Q notation useful throughout this paper. To begin with we will rederive the familiar Fresnel result

$$-r_{p0} = \frac{\tan(\theta_1 - \theta_2)}{\tan(\theta_1 + \theta_2)} \tag{18}$$

for the step profile

$$\begin{aligned}\epsilon_0(z) &= \begin{cases}\epsilon_1, & z<0,\\ \epsilon_2, & z>0\end{cases}\\ &= \tfrac{1}{2}(\epsilon_1+\epsilon_2) - \tfrac{1}{2}(\epsilon_1-\epsilon_2)\,\mathrm{sgn}(z).\end{aligned} \tag{19}$$

For the step (located at the origin),

$$Z_0(z) = z\epsilon_0(z). \tag{20}$$

Continuity of $B_0(Z_0)$ and dB_0/dZ_0, and use of (15) in the form

$$B_0(Z_0) = \begin{cases} e^{iQ_1Z_0} - r_{p0}\, e^{-iQ_1Z_0}, & z<0,\\ \sqrt{\dfrac{\epsilon_2}{\epsilon_1}}\, t_{p0}\, e^{iQ_2Z_0}, & z>0,\end{cases} \tag{21}$$

gives

$$-r_{p0} = \frac{Q_1 - Q_2}{Q_1 + Q_2}, \tag{22}$$

which reduces to (18). The p-wave has zero reflection amplitude when $Q_1 = Q_2$, i.e. at the Brewster angle $\theta_B = \arctan\sqrt{\epsilon_2/\epsilon_1}$. We see directly from (16) that this angle has special significance not only for the step profile, but in general. This is because the wave equation, in the dilated variable Z, links two media with effective wavenumbers Q_i which are equal at this angle (and at no other angle). The analogue in quantum mechanics is reflection at an interface between two media in which the particles have equal potential energy. We illustrate the reason for the near-transparency (for the p-wave) at the Brewster angle in fig. 1, where we show q^2 vs. z and Q^2 vs. Z for the hyperbolic tangent (or Fermi function) profile

$$\begin{aligned}\epsilon(z) &= \tfrac{1}{2}(\epsilon_1+\epsilon_2) - \tfrac{1}{2}(\epsilon_1-\epsilon_2)\tanh(z/2a)\\ &= \frac{\epsilon_1}{1+e^{z/a}} + \frac{\epsilon_2}{1+e^{-z/a}} = \frac{\epsilon_1+\epsilon_2\, e^{z/a}}{1+e^{z/a}}.\end{aligned} \tag{23}$$

For this profile,

$$Z = \tfrac{1}{2}(\epsilon_1+\epsilon_2)z - (\epsilon_1-\epsilon_2)a \log\cosh\left(\frac{z}{2a}\right). \tag{24}$$

At the Brewster angle,

$$K^2 = \left(\frac{\omega}{c}\right)^2 \frac{\epsilon_1\epsilon_2}{\epsilon_1+\epsilon_2}, \quad Q_1^2 = Q_2^2 = \left(\frac{\omega}{c}\right)^2 \frac{1}{\epsilon_1+\epsilon_2}. \tag{25}$$

Thus at θ_B, for a general profile,

$$Q^2 = \left(\frac{\omega}{c}\right)^2 \frac{1}{\epsilon^2}\left\{\epsilon - \frac{\epsilon_1\epsilon_2}{\epsilon_1+\epsilon_2}\right\} \tag{26}$$

and

$$Q^2 - Q_1^2 = Q^2 - Q_2^2 = \left(\frac{\omega}{c}\right)^2 \frac{(\epsilon_1-\epsilon)(\epsilon-\epsilon_2)}{\epsilon^2(\epsilon_1+\epsilon_2)}. \tag{27}$$

This is the analytic expression for the bump in Q^2 at the Brewster angle seen in fig. 1.

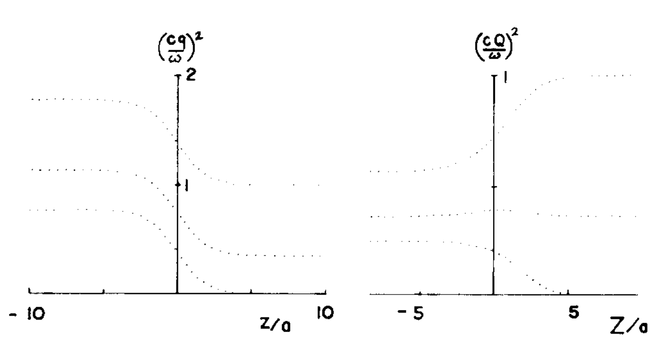

Fig. 1. Reflection of the s-wave and the p-wave. The figure shows $q^2(z)$ and $Q^2(Z)$ for the hyperbolic tangent profile (23), with Z given by (24). The dielectric constants are chosen to approximate the water–air interface: $\epsilon_1 = (4/3)^2$, $\epsilon_2 = 1$. Water is on the left in both diagrams. The upper curve (in each case) is for normal incidence, the middle curve is at the Brewster angle (determined by $Q_1 = Q_2$), and the lower curve is at the critical angle for total interval reflection.

3. Comparison identities for the p-wave

In paper I we derived several identities relating reflection and transmission amplitudes obtained for equations of type (1), to amplitudes obtained with a reference profile. Let the subscript zero denote a reference profile (in later sections this will be taken to be the step profile (19), but here it is arbitrary). The main result in section 2 of I, transcribed to the s-wave, reads

$$r_s = r_{s0} - \frac{1}{2iq_1} \int_{-\infty}^{\infty} dz (q^2 - q_0^2) E E_0, \tag{28}$$

where q^2 and q_0^2 are given by (9), and q, q_0 have the same values q_1 and q_2 deep inside medium 1 and medium 2. This result leads to (11) when the reference profile is taken to be the step profile. We also showed in I that, for real q_1, q_2 and an arbitrary interface,

$$q_2 t_s = q_1 \overleftarrow{t}_s \tag{29}$$

and

$$\overleftarrow{r}_s = -\frac{t_s}{t_s^*} r_s^*. \tag{30}$$

(The backward-pointing arrow indicates amplitudes for a wave incident from medium 2.) These results are implicit in relations derived by Landau and Lifshitz[5]).

In this paper we will derive corresponding results for the p-wave. We note first that (14) is not of the form (1), but may be put in this form in two ways. The first transformation (of the space coordinate) has already been indicated in section 2. But since the new space coordinate Z is a functional of the dielectric profile, each profile has its own Z, and the comparison identities of I cannot be transcribed to the $B(Z)$ form of the p-wave. The second transformation is

$$B = \sqrt{\frac{\epsilon}{\epsilon_1}}\, b. \tag{31}$$

The factor $\epsilon_1^{-1/2}$ is to make the asymptotic form of b the same as that of B in medium 1:

$$e^{iq_1 z} - r_p e^{-iq_1 z} \leftarrow b \rightarrow t_p e^{iq_2 z}. \tag{32}$$

From (14) and (31), $b(z)$ satisfies the equation

$$\frac{d^2 b}{dz^2} + \left[q^2 - \epsilon^{1/2} \frac{d^2 \epsilon^{-1/2}}{dz^2} \right] b = 0, \tag{33}$$

or

$$\frac{\mathrm{d}^2 b}{\mathrm{d}z^2} + \left[q^2 + \frac{1}{2\epsilon}\frac{\mathrm{d}^2\epsilon}{\mathrm{d}z^2} - \frac{3}{4}\left(\frac{1}{\epsilon}\frac{\mathrm{d}\epsilon}{\mathrm{d}z}\right)^2\right] b = 0. \tag{34}$$

The techniques developed in I may be applied to this equation. In particular we find, as in I,

$$q_1(1 - |r_p|^2) = q_2|t_p|^2 \tag{35}$$

$$q_2 t_p = q_1 \overleftarrow{t}_p \tag{36}$$

and

$$\overleftarrow{r}_p = -\frac{t_p}{t_p^*} r_p^* \tag{37}$$

(these relations are for real q_1, q_2 only). We will not give all the comparison identities from which (35)–(37) follow, since these parallel those in I. It is however interesting to examine the analogue of (28), derived from (33):

$$r_p = r_{p0} + \frac{1}{2\mathrm{i}q_1}\int_{-\infty}^{\infty} \mathrm{d}z(\tilde{q}^2 - \tilde{q}_0^2) b b_0, \tag{38}$$

where

$$\tilde{q}^2 = q^2 - \epsilon^{1/2}\frac{\mathrm{d}^2\epsilon^{-1/2}}{\mathrm{d}z^2} = q^2 + \frac{1}{2\epsilon}\frac{\mathrm{d}^2\epsilon}{\mathrm{d}z^2} - \frac{3}{4}\left(\frac{1}{\epsilon}\frac{\mathrm{d}\epsilon}{\mathrm{d}z}\right)^2. \tag{39}$$

When the reference profile ϵ_0 is chosen to be the step function, $\tilde{q}_0^2$ becomes highly singular. It is for this reason that we have preferred to work with an identity based on the following form of (14);

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon}\frac{\mathrm{d}B}{\mathrm{d}z}\right) + \left(\frac{\omega^2}{c} - \frac{K^2}{\epsilon}\right) B = 0. \tag{40}$$

We multiply this equation by B_0, the solution of

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon_0}\frac{\mathrm{d}B_0}{\mathrm{d}z}\right) + \left(\frac{\omega^2}{c^2} - \frac{K^2}{\epsilon_0}\right) B = 0, \tag{41}$$

where

$$\mathrm{e}^{\mathrm{i}q_1 z} - r_{p0}\,\mathrm{e}^{-\mathrm{i}q_1 z} \leftarrow B_0 \rightarrow \sqrt{\frac{\epsilon_2}{\epsilon_1}}\, t_{p0}\,\mathrm{e}^{\mathrm{i}q_2 z} \tag{42}$$

and subtract from this B times (41). The result is

$$B_0\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon}\frac{\mathrm{d}B}{\mathrm{d}z}\right) - B\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon_0}\frac{\mathrm{d}B_0}{\mathrm{d}z}\right) = K^2\left(\frac{1}{\epsilon} - \frac{1}{\epsilon_0}\right) B B_0, \tag{43}$$

or

$$\frac{d}{dz}(B_0C - BC_0) = K^2\left(\frac{1}{\epsilon} - \frac{1}{\epsilon_0}\right)BB_0 - (\epsilon - \epsilon_0)CC_0, \tag{44}$$

where

$$C = \frac{1}{\epsilon}\frac{dB}{dz} = \frac{dB}{dZ}, \quad C_0 = \frac{1}{\epsilon_0}\frac{dB_0}{dz} = \frac{dB_0}{dZ_0}. \tag{45}$$

We now integrate (43) from $-\infty$ to $+\infty$; using (15) we find

$$r_p = r_{p0} + \frac{1}{2iQ_1}\int_{-\infty}^{\infty} dz\left\{\left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right)K^2BB_0 + (\epsilon - \epsilon_0)CC_0\right\}. \tag{46}$$

This identity relates the p-wave reflection amplitudes for two arbitrary profiles. In the next section we shall apply it to determination of r_p to second order in the interface thickness.

We close this section by noting two more interesting identities, obtained by comparing the p-wave with the s-wave. In the first we multiply (14) by the solution of (8) (for the same profile ϵ), and subtract from this B times (8). The result, integrated from $-\infty$ to $+\infty$, gives

$$r_p + r_s = -\frac{1}{2iq_1}\int_{-\infty}^{\infty} dz\left(\frac{d\epsilon}{dz}\right)\left(\frac{1}{\epsilon}\frac{dB}{dz}\right)E. \tag{47}$$

The second identity, obtained from (8) and (33) by the same method, also gives the sum of the reflection amplitudes:

$$\begin{aligned} r_p + r_s &= \frac{-\sqrt{\epsilon_1}}{2iq_1}\int_{-\infty}^{\infty} dz\,\frac{d^2\epsilon^{-1/2}}{dz^2}EB \\ &= \frac{\sqrt{\epsilon_1}}{2iq_1}\int_{-\infty}^{\infty} dz\,\frac{d\epsilon^{-1/2}}{dz}\frac{d}{dz}(EB). \end{aligned} \tag{48}$$

4. The p-wave to second order in the interface thickness

We shall apply (46) with the reference profile being the step profile ϵ_0 (given by (14)). The s-wave results are conditional on the positioning of the step profile to satisfy (6), or

$$\int_{-\infty}^{\infty} dz(\epsilon - \epsilon_0) = 0. \tag{49}$$

We shall continue to use this positioning, which makes the phase of the s-wave zero to second order in qa (when the step is at $z = 0$).

To use (46), we need B and $C = \mathrm{d}B/\mathrm{d}Z$ to first order in the interface thickness in order to get r_p to second order. The factor $\epsilon - \epsilon_0$ in the integrand is non-zero within the interface region, which (according to (19) and (49)) is centred at $z = 0$. Thus we need the expansions of B and C about $z = 0$. The functional form of these expansions can be obtained by converting the second-order differential equation (16) to two coupled first-order differential equations:

$$\frac{\mathrm{d}B}{\mathrm{d}Z} = C, \quad \frac{\mathrm{d}C}{\mathrm{d}Z} = -Q^2 B. \tag{50}$$

From (50) we obtain the integral equations

$$B(Z) = B(0) + \int_0^Z \mathrm{d}Z' C(Z'), \tag{51}$$

$$C(Z) = C(0) - \int_0^Z \mathrm{d}Z' Q^2(Z') B(Z'). \tag{52}$$

The leading terms in the expansion around the origin are

$$B(Z) = B(0) + C(0)Z + \cdots, \tag{53}$$

$$C(Z) = C(0) - B(0) \int_0^Z \mathrm{d}Z' Q^2(Z') + \cdots. \tag{54}$$

These equations give the required functional input into (46), but the constant $B(0)$ has to be evaluated to first order in qa for r_p to be known to second order ($C(0)$ may be replaced by $C_0(0)$ to this order, because of (49)). In the appendix we show that B satisfies the integro-differential equation

$$B(z) = B_0(z) - \int_{-\infty}^{\infty} \mathrm{d}\zeta \left\{ \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right) K^2 B(\zeta) G(z,\zeta) + (\epsilon - \epsilon_0) \frac{1}{\epsilon} \frac{\mathrm{d}B}{\mathrm{d}\zeta} \frac{1}{\epsilon_0} \frac{\partial G}{\partial \zeta} \right\}. \tag{55}$$

The Green's function $G(z, \zeta)$ is defined and evaluated in the appendix. From (55) and (A.3) we find

$$B(0) = B_0(0) - \frac{K^2 B(0)}{\mathrm{i}(Q_1 + Q_2)} \int_{-\infty}^{\infty} \mathrm{d}\zeta \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right) - C(0) \int_{-\infty}^{\infty} \mathrm{d}\zeta (\epsilon - \epsilon_0) Q_0(\zeta)\, \mathrm{sgn}(\zeta)$$
$$+ \mathcal{O}(qa)^2. \tag{56}$$

The term multiplying $C(0)$ is, using (49),

$$Q_1\int_{-\infty}^{0}\mathrm{d}\zeta(\epsilon_0-\epsilon)+Q_2\int_0^{\infty}\mathrm{d}\zeta(\epsilon-\epsilon_0)=(Q_1+Q_2)\int_0^{\infty}\mathrm{d}\zeta(\epsilon-\epsilon_0). \tag{57}$$

Also, from (21) and (22),

$$B_0(0)=\frac{2Q_1}{Q_1+Q_2},\quad C_0(0)=\frac{2\mathrm{i}Q_1Q_2}{Q_1+Q_2} \tag{58}$$

and $B(0)$, $C(0)$ differ from $B_0(0)$, $C_0(0)$ by (at least) terms of order qa. Thus

$$B(0)=\frac{2Q_1}{Q_1+Q_2}\left\{1+\frac{\mathrm{i}K^2D}{Q_1+Q_2}-\mathrm{i}Q_2\Lambda\right\}+\mathcal{O}(qa)^2, \tag{59}$$

where the lengths D and Λ are given by

$$D=\int_{-\infty}^{\infty}\mathrm{d}z\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)=\frac{1}{\epsilon_1\epsilon_2}\int_{-\infty}^{\infty}\mathrm{d}z\,\frac{(\epsilon_1-\epsilon)(\epsilon-\epsilon_2)}{\epsilon}, \tag{60}$$

$$\Lambda=\int_0^{\infty}\mathrm{d}z(\epsilon-\epsilon_0). \tag{61}$$

(The second form of D is obtained using (49)). We now have sufficient information to evaluate r_p to second order. The expansion of r_p in powers of qa is written as

$$r_\mathrm{p}=r_{\mathrm{p}0}+r_{\mathrm{p}1}+r_{\mathrm{p}2}+\cdots. \tag{62}$$

From (46), using (49), (53), (54) and (59), we find the well-known[6,7]) result

$$r_{\mathrm{p}1}=-\frac{2\mathrm{i}Q_1K^2D}{(Q_1+Q_2)^2} \tag{63}$$

and

$$r_{\mathrm{p}2}=\frac{2Q_1}{(Q_1+Q_2)^2}\left\{\frac{K^4D^2}{Q_1+Q_2}+Q_2(\epsilon_1-\epsilon_2)\left[2K^2L^2-\frac{\omega^2}{c^2}l^2\right]\right\}, \tag{64}$$

where

$$2(\epsilon_1-\epsilon_2)L^2=\int_{-\infty}^{\infty}\mathrm{d}z\,z\left(\frac{\epsilon}{\epsilon_0}-\frac{\epsilon_0}{\epsilon}\right)+\int_{-\infty}^{\infty}\mathrm{d}z(\epsilon-\epsilon_0)\int_0^z\frac{\mathrm{d}\zeta}{\epsilon(\zeta)}$$
$$+\int_{-\infty}^{\infty}\mathrm{d}z\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)\int_0^z\mathrm{d}\zeta\,\epsilon(\zeta)-D\Lambda. \tag{65}$$

This combination of integrals may be simplified by using (49) to

$$(\epsilon_1-\epsilon_2)L^2=\int_{-\infty}^{\infty}\mathrm{d}z(\epsilon-\epsilon_0)\left\{\frac{z}{\epsilon}+\int_0^z\frac{\mathrm{d}\zeta}{\epsilon(\zeta)}\right\}. \tag{66}$$

Also of interest is the second-order term in $r_\mathrm{p}/r_\mathrm{s}$ [8]); from (62) and $r_\mathrm{s}=r_{\mathrm{s}0}+r_{\mathrm{s}2}+\mathcal{O}(qa)^3$ we have

$$\frac{r_\mathrm{p}}{r_\mathrm{s}}=\frac{r_{\mathrm{p}0}}{r_{\mathrm{s}0}}+\frac{r_{\mathrm{p}1}}{r_{\mathrm{s}0}}+\frac{1}{r_{\mathrm{s}0}}\left[r_{\mathrm{p}2}-r_{\mathrm{s}2}\frac{r_{\mathrm{p}0}}{r_{\mathrm{s}0}}\right]+\mathcal{O}(qa)^3. \tag{67}$$

From (11) we find

$$\frac{r_{\mathrm{p}0}}{r_{\mathrm{s}0}}r_{\mathrm{s}2}=-\frac{2Q_1Q_2}{(Q_1+Q_2)^2}\left(\frac{\omega^2}{c^2}-\frac{\epsilon_1+\epsilon_2}{\epsilon_1\epsilon_2}K^2\right)(\epsilon_1-\epsilon_2)l^2. \tag{68}$$

Thus, combining (64), (67) and (68),

$$\begin{aligned}\left(\frac{r_\mathrm{p}}{r_\mathrm{s}}\right)_2&=\frac{1}{r_{\mathrm{s}0}}\left[r_{\mathrm{p}2}-r_{\mathrm{s}2}\frac{r_{\mathrm{p}0}}{r_{\mathrm{s}0}}\right]\\&=\frac{q_1+q_2}{q_1-q_2}\frac{2Q_1K^2}{(Q_1+Q_2)^2}\left\{\frac{K^2D^2}{Q_1+Q_2}+Q_2(\epsilon_1-\epsilon_2)\left[2L^2-\frac{\epsilon_1+\epsilon_2}{\epsilon_1\epsilon_2}l^2\right]\right\}.\end{aligned} \tag{69}$$

This term goes to zero at normal incidence, as it must since there is then no physical difference between the s and p waves, so that $r_\mathrm{p}/r_\mathrm{s}=1$, identically.

5. An example

We shall compare the results derived above with the exact solution for the homogeneous dielectric layer[9]); for this problem the dielectric function is a two-step

$$\epsilon(z)=\begin{cases}\epsilon_1, & z<-a,\\ \dfrac{a\epsilon_1+b\epsilon_2}{a+b}, & -a<z<b,\\ \epsilon_2, & z>b.\end{cases} \tag{70}$$

The p-wave reflection amplitude, found by imposing the continuity of B and $\epsilon^{-1}\,\mathrm{d}B/\mathrm{d}z$ (implied by (40)) at $-a$ and b, is

$$-r_\mathrm{p}=\mathrm{e}^{-2\mathrm{i}q_1a}\frac{Q(Q_1-Q_2)c+\mathrm{i}(Q^2-Q_1Q_2)s}{Q(Q_1+Q_2)c-\mathrm{i}(Q^2+Q_1Q_2)s}, \tag{71}$$

where

$$\begin{Bmatrix}c\\ s\end{Bmatrix}=\begin{matrix}\cos\\ \sin\end{matrix}\{q(a+b)\},\quad q^2=\frac{aq_1^2+bq_2^2}{a+b}. \tag{72}$$

The corresponding s-wave reflection amplitude is given by I(31)

$$r_s = e^{-2iq_1 q} \frac{q(q_1 - q_2)c + i(q^2 - q_1 q_2)s}{q(q_1 + q_2)c - i(q^2 + q_1 q_1)s}. \tag{73}$$

The integrals required for r_{p2} are (with ϵ representing the value $(a\epsilon_1 + b\epsilon_2)/(a + b)$)

$$l^2 = (a + b)^2(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)/(\epsilon_1 - \epsilon_2)^2, \tag{74}$$

$$D = (a + b)\frac{(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)}{\epsilon\epsilon_1\epsilon_2}, \tag{75}$$

$$L^2 = (a + b)^2 \frac{(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)}{\epsilon(\epsilon_1 - \epsilon_2)^2}. \tag{76}$$

Thus the second-order contribution to r_p is

$$r_{p2} = \frac{2Q_1(a + b)^2(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)}{(Q_1 + Q_2)^2}\left\{\frac{K^4(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)}{(Q_1 + Q_2)(\epsilon\epsilon_1\epsilon_2)^2} + \frac{Q_2}{\epsilon_1 - \epsilon_2}\left[\frac{2K^2}{\epsilon} - \frac{\omega^2}{c^2}\right]\right\}. \tag{77}$$

This expression checks with the second-order part of (71).

7. The Brewster angles

We saw in section 2 that one would expect near-transparency at the angle of incidence defined by $Q_1 = Q_2$, i.e. determined purely by the bulk properties of the two media:

$$\theta_B(\text{bulk}) = \arctan\sqrt{\frac{\epsilon_2}{\epsilon_1}}. \tag{78}$$

There are other operational definitions of Brewster angles, reducing to (78) in the limit of a step profile, but in general dependent on the interfacial profile characteristics. These are determined by minima in $|r_p|$ or $|r_p/r_s|$, or by the location of the zero of the real part of r_p/r_s. We shall give an expression, to second order in qa, for the angle at which $\text{Re}(r_p/r_s) = 0$: from (67) and the fact that r_{p1} is pure imaginary, we see that this condition requires

$$r_{p0} + r_{p2} - r_{s2}\frac{r_{p0}}{r_{s0}} = 0. \tag{79}$$

We let

$$\theta_B\left(\text{Re}\left(\frac{r_p}{r_s}\right) = 0\right) = \arctan\sqrt{\frac{\epsilon_2}{\epsilon_1}} + \Delta\theta_B. \tag{80}$$

It is apparent from (79) that $\Delta\theta_B = \mathcal{O}(qa)^2$, so the difference in the Brewster angles, to second order in interface thickness, is given by $r_{p0} = -r_{p2}$, or, with $Q_B = (\omega/c)/\sqrt{\epsilon_1 + \epsilon_2}$,

$$\frac{Q_1 - Q_2}{2Q_B} = r_{p2}(\theta_B) + \mathcal{O}(qa)^3. \tag{81}$$

This implies

$$\Delta\theta_B = \frac{2r_{p2}(\theta_B)}{\sqrt{\epsilon_1/\epsilon_2}(\epsilon_1/\epsilon_2 - \epsilon_2/\epsilon_1)} + \mathcal{O}(qa)^3. \tag{82}$$

From (64),

$$r_{p2}(\theta_B) = \frac{\epsilon_1\epsilon_2}{\epsilon_1 + \epsilon_2}\left(\frac{\omega}{c}\right)^2\left[(\epsilon_1 - \epsilon_2)L^2 + \frac{\epsilon_1\epsilon_2}{4}D^2 - \frac{1}{2}\frac{\epsilon_1^2 - \epsilon_2^2}{\epsilon_1\epsilon_2}l^2\right]. \tag{83}$$

The sign of $\Delta\theta_B$ is thus determined by the relative size of the terms in the square bracket.

7. Conclusion

We have developed a variety of techniques for dealing with the electromagnetic p-wave. The second-order ellipsometric formulae derived here appear to be the first explicit results for a general profile expressed as convergent integrals, although there are implicit results in the work of Maclaurin[10]), Rayleigh[6]) and Abelès[11]). The results show that there is a wealth of information in the angular dependence (contained in Q_1, Q_2 and K^2) of r_p and r_p/r_s. Three lengths characterising the profile can be determined from r_{p2}, one of these being obtainable from r_{s2} (see eqs. (11) and (64)), and one (D) from r_{p1}. Two lengths can be determined from $(r_p/r_s)_2$, one of which is D.

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Appendix

An integro-differential equation for the p-wave

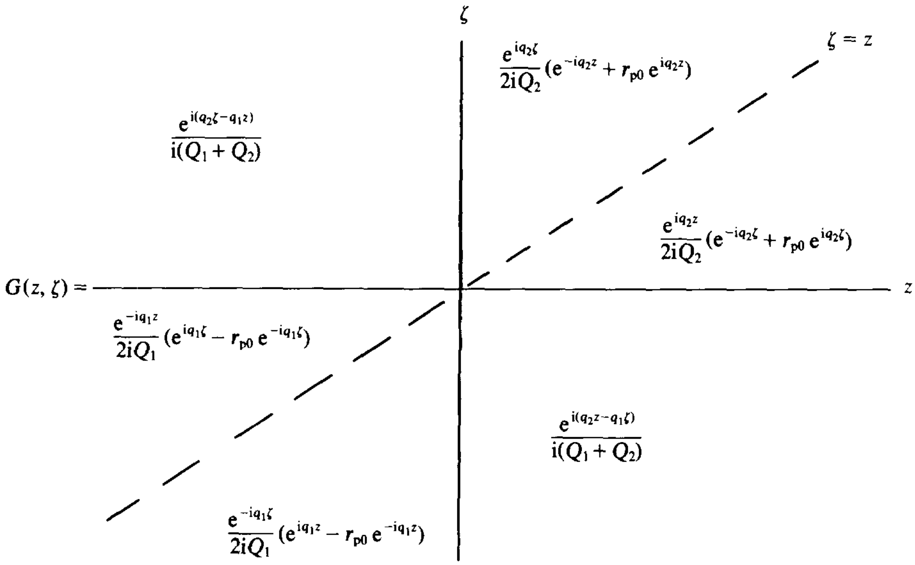
The results given here are closely related to those given in the appendix of I; the discussion will correspondingly be abbreviated. We shall work with the p-wave equation (40), with $v = 1/\epsilon$:

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(v\,\frac{\mathrm{d}B}{\mathrm{d}z}\right)+\left(\frac{\omega^2}{c^2}-vK^2\right)B=0. \tag{A.1}$$

We construct a Green's function $G(z, \zeta)$ satisfying

$$\frac{\partial}{\partial z}\left(v_0\,\frac{\partial G}{\partial z}\right)+\left(\frac{\omega^2}{c^2}-v_0K^2\right)G=\delta(z-\zeta) \tag{A.2}$$

and incorporating the required boundary conditions. This is (cf. I, (A.6))



(A.3)

Now write $v = v_0 + \Delta v$, $B = B_0 + \Delta B$. From (A.1) and the corresponding equation for B_0, ΔB satisfies (with primes denoting $\mathrm{d}/\mathrm{d}z$)

$$(v_0\Delta B')'+\left(\frac{\omega^2}{c^2}-v_0K^2\right)\Delta B+(\Delta v\Delta B')'-K^2\Delta v\Delta B=\Delta_0, \tag{A.4}$$

where

$$\Delta_0 = K^2\Delta vB_0-(\Delta vB_0')'. \tag{A.5}$$

Now expand ΔB as a (functional) power series in Δv:

$$\Delta B = B_1 + B_2 + \cdots. \tag{A.6}$$

We get an infinite set of coupled equations:

$$(v_0B_n')'+\left(\frac{\omega^2}{c^2}-v_0K^2\right)B_n=\Delta_{n-1}, \tag{A.7}$$

where Δ_n is obtained by replacing B_0 by B_n in (A.5). Each of these is formally solved in terms of $G(z, \zeta)$: from (A.7) and (A.2)

$$B_n(z) = \int_{-\infty}^{\infty} \mathrm{d}\zeta G(z, \zeta)\Delta_{n-1}(\zeta). \tag{A.8}$$

Summing these to $n = \infty$, we find

$$\Delta B(z) = \int_{-\infty}^{\infty} \mathrm{d}\zeta G(z, \zeta)\left\{K^2 \Delta v(\zeta) B(\zeta) - \frac{\mathrm{d}}{\mathrm{d}\zeta}\left(\Delta v(\zeta)\frac{\mathrm{d}B}{\mathrm{d}\zeta}\right)\right\}, \tag{A.9}$$

or

$$B(z) = B_0(z) + \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v(\zeta)\left\{K^2 B(\zeta) G(z, \zeta) + \frac{\mathrm{d}B}{\mathrm{d}\zeta}\frac{\partial G}{\partial \zeta}\right\}, \tag{A.10}$$

which proves (55).

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