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INVARIANT FORMULATION OF THE REFLECTION OF LONG WAVES BY INTERFACES

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A theory which calculates reflection amplitudes as perturbation series about a reference profile must obtain results for observables which are invariant to the positioning of the reference profile. We construct a manifestly invariant theory for electromagnetic s and p waves, to second order in the ratio of interface thickness to wavelength. The results are expressed in terms of "integral invariants": combinations of integrals over the difference between the reference and the actual dielectric functions, which are invariant to their relative positioning. To second order in the interface thickness, $|r_s|^2$ is characterized by one second order invariant (i_2), while $|r_p|^2$ and r_p/r_s are each characterized by a first order invariant ($\mathscr{I}_1$) and two second order invariants (i_2 and j_2).

The theory given has greater generality than previous perturbation theories, applying to reflections from absorbing interfaces and/or substrates, and to reflections from a thin film between like media (such as a soap film in air). In the latter case we find that r_p/r_s is zero (to lowest order) at a certain angle.

1. Introduction

When the thickness of an interface is small compared to the wavelength of light incident upon it, we expect the reflection amplitudes for the s and p polarizations to be well represented by the first few terms of series in the ratio of the interface thickness to the wavelength of light, with the zeroth terms given by the Fresnel formulae. Corrections to the Fresnel formulae up to second order have been obtained in refs. 1 and 2 (to be designated I and II in this paper); the results may be interpreted in terms of lengths characterizing the interface, these lengths being integrals over the difference between the actual dielectric profile $\epsilon(z)$, and the step profile $\epsilon_0(z)$, which takes the values ϵ_1 for $z<0$ and for ϵ_2 for $z>0$. In the theory as developed so far, it was convenient to simplify the analysis by relative positioning of the actual and reference profiles so as to make

$$\int_{-\infty}^{\infty} dz[\epsilon(z)-\epsilon_0(z)]=0\,. \tag{1}$$

Such positioning (the equal-area rule, see fig. 1 of I) is always possible when

$\epsilon_1 \neq \epsilon_2$ and ϵ is real everywhere. However, for reflection at an interface between two like media ($\epsilon_1 = \epsilon_2$), or in the presence of absorption (ϵ complex), the condition (1) can no longer be guaranteed.

In this paper we shall generalize the theory by removing the constraint (1). At the same time we recast the results in such a way that the absolute magnitudes of the reflection amplitudes, and their phase difference, are explicitly invariant with respect to the relative positioning of ϵ and ϵ_0. This is made possible by the theory of *integral invariants*, developed in the appendices, which appears to have general application to the solution of problems by the use of a reference function whose positioning is not fixed by physical constraints.

2. First order results

To introduce our techniques and notation, we shall briefly rederive the first order correction to the Fresnel formulae. This result, usually credited to Drude[3]), was apparently first obtained by Lorenz[4]): Rayleigh[5]) gives a derivation and references to the earlier work of Lorenz, Van Ryn, Drude, Schott and Maclaurin.

For the s wave, the constraint (1) is not used in the perturbation theory developed in the appendix of paper I. From I-(A.8) we have

$$r_{s1} = \frac{2iq_1\omega^2/c^2}{(q_1+q_2)^2} \int_{-\infty}^{\infty} dz[\epsilon(z) - \epsilon_0(z)] \,, \tag{2}$$

where q_1 and q_2 are the normal components for the wavenumber in media 1 and 2, ω is the angular frequency and c is the speed of light in vacuum, and r_{s1} denotes the first order term in the expansion of r_s in powers of the interface thickness.

For the p wave, we use the comparison identity II-(46):

$$r_p = r_{p0} + \frac{1}{2iQ_1} \int_{-\infty}^{\infty} dz \left\{ \left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right) K^2 BB_0 + (\epsilon - \epsilon_0) CC_0 \right\} , \tag{3}$$

where $K^2 = \epsilon_1\omega^2/c^2 - q_1^2 = \epsilon_2\omega^2/c^2 - q_2^2$, $Q_1 = q_1/\epsilon_1$, and $C = (1/\epsilon)\, dB/dz$, $C_0 = (1/\epsilon_0)\, dB_0/dz$. To first order in the interface thickness, it suffices to replace BB_0

and CC_0 in the integrand by $B_0^2(0)$ and $C_0^2(0)$, where (II-(58))

$$B_0(0) = \frac{2Q_1}{Q_1 + Q_2}, \quad C_0(0) = \frac{2iQ_1Q_2}{Q_1 + Q_2}. \tag{4}$$

We obtain

$$r_{p1} = \frac{-2iQ_1}{(Q_1 + Q_2)^2}\left\{\frac{K^2}{\epsilon_1\epsilon_2}\Lambda_1 - Q_2^2\lambda_1\right\}, \tag{5}$$

where

$$\lambda_1 = \int_{-\infty}^{\infty} dz(\epsilon - \epsilon_0), \quad \Lambda_1 = \epsilon_1\epsilon_2 \int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right). \tag{6}$$

In appendix A we show that, though both λ_1 and Λ_1 are in general dependent on the relative placement of the dielectric function profiles ϵ and ϵ_0, the difference $\mathscr{I}_1 = \Lambda_1 - \lambda_1$ is independent of this placement (is an invariant). The ratio r_p/r_s must not depend on an arbitrary choice of such placement. We have

$$\frac{r_p}{r_s} = \frac{r_{p0} + r_{p1} + \cdots}{r_{s0} + r_{s1} + \cdots} = \frac{r_{p0}}{r_{s0}}\left(1 + \frac{r_{p1}}{r_{p0}} - \frac{r_{s1}}{r_{s0}} + \cdots\right). \tag{7}$$

From (2), (5) and

$$r_{s0} = \frac{q_1 - q_2}{q_1 - q_2}, \quad -r_{p0} = \frac{Q_1 - Q_2}{Q_1 + Q_2}, \tag{8}$$

we find

$$\frac{r_{s1}}{r_{s0}} = \frac{2iq_1\lambda_1}{\epsilon_1 - \epsilon_2}, \quad \frac{r_{p1}}{r_{p0}} = \frac{2iQ_1}{Q_1^2 - Q_2^2}\frac{K^2}{\epsilon_1\epsilon_2}(\Lambda_1 - \lambda_1) + \frac{r_{s1}}{r_{s0}}. \tag{9}$$

In obtaining the second equality in (9) we have used the relation

$$\frac{K^2}{\epsilon_1\epsilon_2} = \frac{\epsilon_1 Q_1^2 - \epsilon_2 Q_2^2}{\epsilon_1 - \epsilon_2}. \tag{10}$$

We have thus verified that the first order part of r_p/r_s is invariant, being proportional to $\mathscr{I}_1$. Note that $\mathscr{I}_1 = \Lambda_1 - \lambda_1$ can be written in a manifestly invariant (and more familiar[6]) form by means of the identity

$$\epsilon_1\epsilon_2 \int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0} - \frac{1}{\epsilon}\right) - \int_{-\infty}^{\infty} dz(\epsilon - \epsilon_0) = \int_{-\infty}^{\infty} dz\, \frac{(\epsilon_1 - \epsilon)(\epsilon - \epsilon_2)}{\epsilon}\,. \tag{11}$$

In the special case where ϵ_0 is constant ($\epsilon_1 = \epsilon_2$), the step has disappeared and the question of its positioning does not arise. Then λ_1 and Λ_1 are separately invariant. The Fresnel reflection amplitudes are now zero, and the "first order" part of r_p/r_s becomes zero order:

$$\frac{r_p}{r_s} = \frac{r_{p1}}{r_{s1}} + \cdots = 1 - \frac{K^2}{\epsilon_0\omega^2/c^2}\frac{\Lambda_1 + \lambda_1}{\lambda_1} + \cdots\,. \tag{12}$$

The case $\epsilon_0 =$ constant will be discussed in more detail in section 4.

3. Second order results

The s wave result can again be read off from the perturbation theory of paper I. From I-(A.8) and I-(A.13) we have

$$r_{s2} = -\frac{4q_1q_2\omega^2/c^2}{(q_1+q_2)^2}\int_{-\infty}^{\infty} dz\, z(\epsilon - \epsilon_0) - \frac{2q_1\omega^4/c^4}{(q_1+q_2)^3}\left(\int_{-\infty}^{\infty} dz(\epsilon - \epsilon_0)\right)^2\,. \tag{13}$$

In terms of λ_1 of eq. (6) and

$$\lambda_2 = \int_{-\infty}^{\infty} dz\, z(\epsilon - \epsilon_0) \tag{14}$$

we have

$$r_{s2} = \frac{-2q_1\omega^2/c^2}{(q_1+q_2)^2}\left\{2q_2\lambda_2 + \frac{\omega^2/c^2}{q_1+q_2}\lambda_1^2\right\}\,. \tag{15}$$

Consider the absolute square of the reflection amplitude:

$$\begin{aligned}|r|^2 &= |r_0 + r_1 + r_2 + \cdots|^2 \\ &= |r_0|^2 + 2\,\mathrm{Re}(r_0^* r_1) + \{|r_1|^2 + 2\,\mathrm{Re}(r_0^* r_2)\} + \cdots.\end{aligned} \tag{16}$$

Here we restrict ourselves to real ϵ and real q_2 (this excludes total internal reflection). Then, for both the s and p waves, r_0 is real and r_1 is purely imaginary, so the lowest correction to r_0^2 is the second order term in the curly bracket of (16). This must be invariant. From (2) and (15) we find

$$\{|r_{s1}|^2 + 2r_{s0}r_{s2}\} = -\frac{4q_1q_2\omega^4/c^4}{(q_1+q_2)^4}\,[2(\epsilon_1-\epsilon_2)\lambda_2 - \lambda_1^2]\,. \tag{17}$$

In appendix A we show that the quantity in the square brackets is an invariant, the first in an infinite set involving the λ_n.

The second order p wave can be obtained from the theory developed in paper II, but requires substantial additional work. We again use the comparison identity (3). The second order contribution r_{p2} is obtained by evaluating the integrand in (3) to first order. From II-(53) we have

$$BB_0 = B_0^2(0) + B_0(0)[\Delta B(0) + C_0(0)(Z_0 + Z)] + \cdots, \tag{18}$$

where $\Delta B(0) = B(0) - B_0(0)$ is given by II-(56) (corrected by dividing the second integral by $(Q_1 + Q_2)$):

$$\begin{aligned}\Delta B(0) &= \left\{\frac{\mathrm{i}K^2}{\epsilon_1\epsilon_2}\Lambda_1 B_0(0) - C_0(0)\int_{-\infty}^{\infty} \mathrm{d}z(\epsilon-\epsilon_0)Q_0(z)\,\mathrm{sgn}(z)\right\}(Q_1+Q_2)^{-1} + \cdots \\ &= \frac{2\mathrm{i}Q_1}{(Q_1+Q_2)^2}\left\{\frac{K^2}{\epsilon_1\epsilon_2}\Lambda_1 + Q_1Q_2\lambda_1 - Q_2(Q_1+Q_2)\lambda_1^+\right\} + \cdots,\end{aligned} \tag{19}$$

where

$$\lambda_1^+ = \int_0^{\infty} \mathrm{d}z(\epsilon-\epsilon_0)\,. \tag{20}$$

The dilated variables Z_0 and Z are defined by II-(17):

$$Z_0 = z\epsilon_0(z)\,, \quad Z = \int_0^z d\zeta\, \epsilon(\zeta)\,. \tag{21}$$

Thus the second order part of r_p arising out of the BB_0 term in the integrand of (3) is

$$r^B_{p2} = \frac{2K^2 Q_1 Q_2}{(Q_1+Q_2)^3}\left[\frac{\Lambda_1}{\epsilon_1\epsilon_2}\left\{\frac{K^2}{Q_2}\frac{\Lambda_1}{\epsilon_1\epsilon_2} + Q_1\lambda_1 - (Q_1+Q_2)\lambda_1^+\right\}\right.$$

$$\left. + (Q_1+Q_2)\int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0}+\frac{1}{\epsilon}\right)(Z_0+Z)\right]. \tag{22}$$

We now evaluate r^C_{p2}, the second order contribution to r_p arising out of the CC_0 term in the integrand of (3). We use II-(54) to obtain

$$CC_0 = C_0^2(0) + C_0(0)\left[\Delta C(0) - B_0(0)\left(\int_0^{Z_0} + \int_0^{Z}\right)\right] + \cdots, \tag{23}$$

where $\int_0^Z$ denotes

$$\int_0^Z dZ' Q^2(Z') = \int_0^z \frac{d\zeta}{\epsilon(\zeta)}\left[\epsilon(\zeta)\frac{\omega^2}{c^2} - K^2\right] = z\frac{\omega^2}{c^2} - K^2\int_0^z \frac{d\zeta}{\epsilon(\zeta)}, \tag{24}$$

and in $\int_0^{Z_0}$ the last integral in (24) is replaced by $z/\epsilon_0(z)$. Thus

$$CC_0 = C_0^2(0) + C_0(0)\left[\Delta C(0) - B_0(0)\left(2z\frac{\omega^2}{c^2} - K^2\left\{\frac{z}{\epsilon_0(z)} + \int_0^z \frac{d\zeta}{\epsilon(\zeta)}\right\}\right)\right] + \cdots. \tag{25}$$

The $\Delta C(0) = C(0) - C_0(0)$ term may be evaluated by differentiating the integrodifferential equation II-(55), care being taken to include the $-\epsilon_0(z)\delta(z-\zeta)$ contribution from $\partial^2 G/\partial z\delta\zeta$. We find

$$\Delta C(0) = \frac{2Q_1Q_2}{(Q_1+Q_2)^2}\left\{K^2Q_1\int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)Q_0^{-1}(z)\,\mathrm{sgn}(z) - Q_1Q_2\lambda_1\right\}$$

$$= \frac{2Q_1Q_2}{(Q_1+Q_2)^2}\left\{\frac{K^2}{\epsilon_1\epsilon_2}\left[\left(1+\frac{Q_1}{Q_2}\right)\Lambda_1^\dagger - \Lambda_1\right] - Q_1Q_2\lambda_1\right\}, \tag{26}$$

where

$$\Lambda_1^\dagger = \epsilon_1\epsilon_2\int_0^\infty dz\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right). \tag{27}$$

We thus have

$$r_{p2}^C = \frac{2Q_1Q_2}{(Q_1+Q_2)^3}\left[\lambda_1\frac{K^2}{\epsilon_1\epsilon_2}\{(Q_1+Q_2)\Lambda_1^\dagger - Q_2\Lambda_1\} - Q_1Q_2^2\lambda_1^2\right.$$

$$\left. - (Q_1+Q_2)\left\{2\frac{\omega^2}{c^2}\lambda_2 - K^2\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\left[\frac{z}{\epsilon_0}+\int_0^z\frac{d\zeta}{\epsilon(\zeta)}\right]\right\}\right]. \tag{28}$$

From (22) and (28) we have

$$r_{p2} = \frac{2Q_1Q_2}{(Q_1+Q_2)^3}\left[\frac{K^4}{Q_2}\left(\frac{\Lambda_1}{\epsilon_1\epsilon_2}\right)^2\right.$$

$$\left. + K^2\left\{(Q_1-Q_2)\frac{\lambda_1\Lambda_1}{\epsilon_1\epsilon_2} + (Q_1+Q_2)J\right\} - Q_1Q_2^2\lambda_1^2 - 2(Q_1+Q_2)\frac{\omega^2}{c^2}\lambda_2\right], \tag{29}$$

where

$$J = \frac{\lambda_1\Lambda_1^\dagger - \lambda_1^\dagger\Lambda_1}{\epsilon_1\epsilon_2} + \int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\left[\frac{z}{\epsilon}+\frac{z}{\epsilon_0}+\frac{1}{\epsilon\epsilon_0}\int_0^z d\zeta\,\epsilon(\zeta) + \int_0^z\frac{d\zeta}{\epsilon(\zeta)}\right]. \tag{30}$$

We will first check that the second order contribution to $|r_p|^2$ is an invariant. This contribution is (cf. (16) and the discussion following)

$$|r_{p1}|^2 + 2r_{p0}r_{p0} = \frac{4Q_1Q_2}{(Q_1+Q_2)^4}\left\{\left(\frac{K^2}{\epsilon_1\epsilon_2}\right)^2\Lambda_1^2 - (Q_1^2+Q_2^2)\frac{K^2}{\epsilon_1\epsilon_2}\lambda_1\Lambda_1 + Q_1^2Q_2^2\lambda_1^2\right.$$

$$\left. + 2(Q_1^2-Q_2^2)\frac{\omega^2}{c^2}\lambda_2 - (Q_1^2-Q_2^2)K^2J\right\}. \tag{31}$$

The coefficient of $(K^2/\epsilon_1\epsilon_2)^2$ inside the curly bracket in (31) is

$$\lambda_1^2+\left(\frac{\epsilon_1}{\epsilon_2}+\frac{\epsilon_2}{\epsilon_1}\right)\lambda_1\Lambda_1+\Lambda_1^2+(\epsilon_2^2-\epsilon_1^2)J$$
$$=(\epsilon_1^2-\epsilon_2^2)\left[\left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)(\lambda_2+\Lambda_2)-J\right]-\left[i_2+I_2+\left(\frac{\epsilon_1}{\epsilon_2}+\frac{\epsilon_2}{\epsilon_1}\right)\mathcal{I}_2\right], \quad (32)$$

where we have used (A.5), (A.14) and (A.15). The coefficient of $(K^2/\epsilon_1\epsilon_2)\omega^2/c^2$ is similarly expressible as

$$(\epsilon_1-\epsilon_2)\left[J-\left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)(\lambda_2+\Lambda_2)\right]+\left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)(i_2+\mathcal{I}_2). \quad (33)$$

Finally, the coefficient of ω^4/c^4 may be written in a manifestly invariant form as $-\epsilon_1\epsilon_2 i_2$. Thus the second order contribution to $|r_p|^2$ is an invariant if

$$J_2=J-\left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)(\lambda_2+\Lambda_2) \quad (34)$$

is an invariant. This invariance is demonstrated in appendix B.

We next examine the second order contribution to r_p/r_s.

This is

$$(r_p/r_s)_2=\left\{r_{p2}r_{s0}-r_{s2}r_{p0}-\frac{r_{s1}}{r_{s0}}(r_{p1}r_{s0}-r_{s1}r_{p0})\right\}\Big/r_{s0}^2. \quad (35)$$

Using the identities

$$(q_1\mp q_2)(Q_1\pm Q_2)=\left(\frac{1}{\epsilon_2}-\frac{1}{\epsilon_1}\right)(K^2\pm q_1q_2), \quad (36)$$

$$Q_1^2-Q_2^2=\left(\frac{1}{\epsilon_2}-\frac{1}{\epsilon_1}\right)\left[\left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)K^2-\frac{\omega^2}{c^2}\right] \quad (37)$$

and

$$\epsilon_1\epsilon_2(Q_1+Q_2)\frac{\omega^2}{c^2}=(q_1+q_2)(K^2+q_1q_2), \quad (38)$$

we find

$$r_{s0}\left(\frac{r_p}{r_s}\right)_2 = \frac{2Q_1(K^2/\epsilon_1\epsilon_2)^2\mathscr{I}_1^2}{(Q_1+Q_2)^3} + \frac{2Q_1Q_2K^2}{(Q_1+Q_2)^2}\left[J_2 + \frac{\epsilon_1+\epsilon_2}{\epsilon_1\epsilon_2(\epsilon_1-\epsilon_2)}(\mathscr{I}_2 - i_2)\right]. \quad (39)$$

We have thus verified that the second order contribution to r_p/r_s is invariant. In addition we see from (39) that this contribution goes to zero with K^2, as it must since there is no physical difference between the s and p waves at normal incidence, for which $r_p/r_s = 1$ identically.

4. Reflection by an inhomogeneous film between two like media

Consider a soap film in air, or two slabs of glass glued together. There is reflection from the soap film, or the glue, due to the variation in the dielectric function. But there is no step in the dielectric function: $\epsilon_1 = \epsilon_2$. An analogous case in quantum mechanics is the reflection of electrons at an oxide barrier between two pieces of the same metal. We will examine the results of second-order theory in this special but important case. Let ϵ_0 now denote the common value of ϵ_1 and ϵ_2, q_0 the common value of q_1 and q_2, etc. The zeroth-order reflection amplitudes are now zero ($q_1 = q_2$ and $Q_1 = Q_2$). The first order reflection amplitudes are (from (2) and (5))

$$r_{s1} = \frac{i\omega^2/c^2}{2q_0}\lambda_1 \quad (40)$$

and

$$r_{p1} = \frac{-i}{2Q_0}\left\{\frac{K^2}{\epsilon_0^2}\Lambda_1 - Q_0^2\lambda_1\right\}$$
$$= \frac{-i\omega^2/c^2}{2q_0}\{\Lambda_1 \sin^2\theta_0 - \lambda_1\cos^2\theta_0\}. \quad (41)$$

The second order reflection amplitudes are (from (15) and (29))

$$r_{s2} = -\frac{\omega^2}{c^2}\left\{\lambda_2 + \frac{\omega^2/c^2}{4q_0^2}\lambda_1^2\right\} \quad (42)$$

and

$$r_{p2} = \frac{K^4\Lambda_1^2}{4\epsilon_0^2q_0^2} + \frac{1}{2}K^2J - \frac{1}{4}Q_0^2\lambda_1^2 - \frac{\omega^2}{c^2}\lambda_2. \quad (43)$$

We noted before that λ_1 and Λ_1 are separately invariant when $\epsilon_1 = \epsilon_2$. When $r_0 = 0$ the second order contribution to the square of the modulus of the reflection amplitude is $|r_1|^2$, and from (40) and (41) the reflected intensities are invariant to this order. The ratio r_p/r_s becomes (when r_{p0} and r_{s0} are zero, and terms to second order are included)

$$\frac{r_{p1}+r_{p2}}{r_{s1}+r_{s2}} = \frac{r_{p1}}{r_{s1}} + \frac{r_{p2}r_{s1} - r_{s2}r_{p1}}{r_{s1}^2} + \cdots . \tag{44}$$

The ratio of first order terms is (from (40) and (41))

$$\frac{r_{p1}}{r_{s1}} = \cos^2\theta_0 - \frac{\Lambda_1}{\lambda_1}\sin^2\theta_0 . \tag{45}$$

This ratio is zeroth order in the interface thickness, and correctly tends to unity as θ_0, the angle of incidence and refraction, tends to zero.

When λ_1 and Λ_1 have the same sign, as would normally be the case, there is an angle at which the film is transparent to the p wave (to the lowest order). This angle is the arctangent of the square root of the ratio

$$\left(\frac{\lambda_1}{\Lambda_1}\right)_{\epsilon_1=\epsilon_2} = \frac{\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)/\epsilon_0}{\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)/\epsilon} . \tag{46}$$

Thus, for thin films between like media, there is an analogue of the Brewster angle. (For four possible definitions of the Brewster angle, and a relationship between two of these, see section 7 of II).

An important special case is that of a uniform thin film of (constant) dielectric function ϵ, located between z_1 and $z_2 = z_1 + \Delta z$ in a medium of dielectric function ϵ_0. Then, from I-(31) and II-(73) we have

$$r_s = e^{2iq_0z_1}\frac{i(q^2-q_0^2)\tau}{2qq_0 - i(q^2+q_0^2)\tau} \tag{47}$$

and

$$-r_p = e^{2iq_0z_1}\frac{i(Q^2-Q_0^2)\tau}{2QQ_0 - i(Q^2+Q_0^2)\tau}, \tag{48}$$

where

$$q^2 = \epsilon \frac{\omega^2}{c^2} - K^2, \quad Q = q/\epsilon, \quad \tau = \tan q\Delta z. \tag{49}$$

Thus

$$\frac{r_p}{r_s} = \left[1 - \left(\frac{cK}{\omega}\right)^2 \frac{\epsilon + \epsilon_0}{\epsilon\epsilon_0}\right]\left\{\frac{1 - \frac{i}{2}\left(\frac{q}{q_0} + \frac{q_0}{q}\right)\tau}{1 - \frac{i}{2}\left(\frac{Q}{Q_0} + \frac{Q_0}{Q}\right)\tau}\right\}. \tag{50}$$

The square bracket in (50) is equal to $\cos^2\theta_0 - (\epsilon_0/\epsilon)\sin^2\theta_0$, and is zero at $\theta_0 = \arctan\sqrt{\epsilon/\epsilon_0}$, which is the same as the (bulk) Brewster angle for light incident from medium with dielectric constant ϵ_0 onto a medium of dielectric constant ϵ. It follows that a uniform film between two like media is always transparent to the p wave at the same angle, irrespective of its thickness.

A non-uniform film, on the other hand, is transparent only to lowest order in its thickness, as can be seen from (44). We have, using (40–43),

$$r_{p2}r_{s1} - r_{s2}r_{p1} = \frac{i(\omega^2/c^2)K^2}{2q_0}\left\{\frac{\lambda_1\Lambda_1}{4\epsilon_0 q_0^2}\left[\frac{K^2\Lambda_1}{\epsilon_0} - \frac{\omega^2}{c^2}\lambda_1\right] + \frac{1}{2}J\lambda_1 - \frac{\lambda_2}{\epsilon_0}(\lambda_1 + \Lambda_1) + \frac{\lambda_1^3}{4\epsilon_0^2}\right\}. \tag{51}$$

This term is zero at $\theta_0 = 0$, but not (in general) at $\theta_0 = \arctan\sqrt{\lambda_1/\Lambda_1}$. To verify the invariance of the second order term, we note that when $\epsilon_1 = \epsilon_2$, λ_1 and Λ_1 are separately invariant, and (on using (A.3), (A.13) and the invariance of J_2) $\epsilon_0\lambda_1 J - 2\lambda_2(\lambda_1 + \Lambda_1)$ transforms into itself.

5. Summary, and comparison with earlier work

We have developed a formalism which enables experimentally accessible reflection properties to be expressed in terms of invariants (combinations of integrals involving the difference between the dielectric profile and a reference step profile). Explicit results are given up to the second order in the interfacial thickness. For real $\epsilon(z)$ and real q_2 these are

$$|r_s|^2 = r_{s0}^2 - \frac{4q_1q_2}{(q_1+q_2)^4}\frac{\omega^4}{c^4} i_2 + \cdots, \tag{52}$$

$$|r_{\mathrm{p}}|^2 = r_{\mathrm{p0}}^2 - \frac{4Q_1Q_2}{\epsilon_1\epsilon_2(Q_1+Q_2)^4}\left\{\frac{\omega^4}{c^4}i_2 - \frac{\omega^2}{c^2}K^2\left[(\epsilon_1-\epsilon_2)J_2 + \left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)(i_2+\mathscr{I}_2)\right] + \frac{K^4}{\epsilon_1\epsilon_2}\left[(\epsilon_1^2-\epsilon_2^2)J_2 + i_2 + I_2 + \left(\frac{\epsilon_1}{\epsilon_2}+\frac{\epsilon_2}{\epsilon_1}\right)\mathscr{I}_2\right]\right\} + \cdots . \tag{53}$$

When $\epsilon_1 \neq \epsilon_2$ we also have

$$r_{\mathrm{s0}}\left(\frac{r_{\mathrm{p}}}{r_{\mathrm{s}}}\right)_1 = \frac{r_{\mathrm{p1}}r_{\mathrm{s0}} - r_{\mathrm{s1}}r_{\mathrm{p0}}}{r_{\mathrm{s0}}} = -\frac{2\mathrm{i}Q_1}{(Q_1+Q_2)^2}\frac{K^2}{\epsilon_1\epsilon_2}\mathscr{I}_1 . \tag{54}$$

Note that the reality of ϵ has not been assumed in the derivation, so that (54) remains valid in the presence of absorption.

When $\epsilon_1 = \epsilon_2$ (and thus $q_1 = q_2$ etc.), the lowest order term in $r_{\mathrm{p}}/r_{\mathrm{s}}$ becomes

$$\frac{r_{\mathrm{p1}}}{r_{\mathrm{s1}}} = \cos^2\theta_0 - \frac{\Lambda_1}{\lambda_1}\sin^2\theta_0 \tag{45}$$

which is now zeroth order in the interface thickness. A film between two like media is thus transparent to the p wave (to lowest order) at the angle

$$\theta = \arctan\sqrt{\frac{\lambda_1}{\Lambda_1}} . \tag{55}$$

Our earlier work[1,2]) on reflection was based on the simplifying assumption $\lambda_1 = 0$ (and thus excluded the $\epsilon_1 = \epsilon_2$ case). From I-(23) and I-(26), when $\lambda_1 = 0$,

$$r_{\mathrm{s}} = r_{\mathrm{s0}}\left\{1 - 2q_1q_2l^2 + \cdots\right\}, \tag{56}$$

where

$$l^2 = \frac{2\lambda_2}{\epsilon_1 - \epsilon_2} . \tag{57}$$

The length l is related to i_2 by

$$i_2 = (\epsilon_1 - \epsilon_2)^2 l^2 \quad (\text{when } \lambda_1 = 0) . \tag{58}$$

From II-(64) (again with $\lambda_1 = 0$)

$$r_{p2} = \frac{2Q_1}{(Q_1+Q_2)^2}\left\{\frac{K^4D^2}{Q_1+Q_2} + Q_2(\epsilon_1-\epsilon_2)\left[2K^2L^2 - \frac{\omega^2}{c^2}l^2\right]\right\}, \tag{59}$$

where $D = \int_{-\infty}^{\infty} dz(1/\epsilon_0 - 1/\epsilon)$. On letting $\lambda_1 \to 0$ in (29) we find

$$r_{p2} \to \frac{2Q_1}{(Q_1+Q_2)^2}\left\{\frac{K^2(\Lambda_1/\epsilon_1\epsilon_2)^2}{Q_1+Q_2} + Q_2\left[K^2J - 2\frac{\omega^2}{c^2}\lambda_2\right]\right\}. \tag{60}$$

The length L is thus related to J by

$$J = 2(\epsilon_1-\epsilon_2)L^2 \qquad (\text{when } \lambda_1 = 0). \tag{61}$$

With II-(66) this implies

$$J = 2\int_{-\infty}^{\infty} dz[\epsilon(z) - \epsilon_0(z)]\left\{\frac{z}{\epsilon(z)} + \int_0^z \frac{d\zeta}{\epsilon(\zeta)}\right\} \quad (\text{when } \lambda_1 = 0). \tag{62}$$

These relations are useful in the evaluation of second order invariants.

In the earlier work we found that s and p wave reflections were completely characterized to second order in the interface thickness by three lengths, D, l and L. This is in apparent distinction to the present work, where we have one first order invariant $\mathcal{I}_1$, and three second order invariants (i_2, I_2 and J_2) [we do not count $\mathcal{I}_2$ as an independent invariant, since $\mathcal{I}_2 = \frac{1}{2}(i_2 + I_2 + \mathcal{I}_1^2)$]. However, we note that in the second order term of $|r_p|^2$ (eq. (53)), J_2, i_2, I_2 and $\mathcal{I}_1$ occur together in the combination

$$j_2 = (\epsilon_1-\epsilon_2)J_2 + \left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)\mathcal{I}_2. \tag{63}$$

In terms of j_2, (53) may be rewritten as

$$|r_p|^2 = r_{p0}^2 - \frac{4Q_1Q_2}{\epsilon_1\epsilon(Q_1+Q_2)^4}\left\{\frac{\omega^4}{c^4}i_2 - \frac{\omega^2}{c^2}K^2\left[j_2 + \left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)i_2\right] + \frac{K^4}{\epsilon_1\epsilon_2}[(\epsilon_1+\epsilon_2)j_2 - \mathcal{I}_1^2]\right\} + \cdots \tag{64}$$

TABLE I

First and second order invariants for five profiles. The first three interfaces extend from z_1 to $z_1 + \Delta z$ (z_1 arbitrary); for the exponential and hyperbolic tangent profiles Δz is a measure of the interface thickness (more details are given in appendix C). Note that the invariants are symmetric with respect to the interchange of ϵ_1 and ϵ_2, and are non-negative for monotonic profiles.

Profile	$\mathcal{I}_1/\Delta z$	$i_2/(\Delta z)^2$	$j_2/(\Delta z)^2$	References
two-step	$\frac{(\epsilon_1-\epsilon)(\epsilon-\epsilon_2)}{\epsilon}$	$(\epsilon_1-\epsilon)(\epsilon-\epsilon_2)$	$2(\epsilon_1-\epsilon)(\epsilon-\epsilon_2)/\epsilon$	1, 2
linear	$\frac{1}{2}(\epsilon_1+\epsilon_2)-\frac{\epsilon_1\epsilon_2}{\epsilon_1-\epsilon_2}\log\frac{\epsilon_1}{\epsilon_2}$	$\frac{1}{12}(\epsilon_1-\epsilon_2)^2$	$\frac{1}{2}(\epsilon_1+\epsilon_2)-\frac{\epsilon_1\epsilon_2}{\epsilon_1-\epsilon_2}\log\frac{\epsilon_1}{\epsilon_2}$	6, 1
Rayleigh	$\frac{2}{3}(\epsilon_1-2\sqrt{\epsilon_1\epsilon_2}+\epsilon_2)$	$\frac{(\epsilon_1-\epsilon_2)^2\epsilon_1\epsilon_2}{\epsilon_1-2\sqrt{\epsilon_1\epsilon_2}+\epsilon_2}\left\{\frac{\log\epsilon_1/\epsilon_2}{\epsilon_1-\epsilon_2}-\frac{4}{\epsilon_1+2\sqrt{\epsilon_1\epsilon_2}+\epsilon_2}\right\}$	$\frac{2}{3}(\epsilon_1-2\sqrt{\epsilon_1\epsilon_2}+\epsilon_2)$	9
exponential	$\epsilon_1\log\frac{\epsilon_1+\epsilon_2}{2\epsilon_1}+\epsilon_2\log\frac{\epsilon_1+\epsilon_2}{2\epsilon_1}$	$2(\epsilon_1-\epsilon_2)^2$	$2(\epsilon_1-\epsilon_2)\left\{\log\frac{\epsilon_1}{\epsilon_2}+\int_{(\epsilon_2-\epsilon_1)/2\epsilon_1}^{(\epsilon_1-\epsilon_2)/2\epsilon_2}\mathrm{d}x\,\frac{\log(1+x)}{x}\right\}$	6,1
tanh	$(\epsilon_1-\epsilon_2)\log\frac{\epsilon_1}{\epsilon_2}$	$\frac{\pi^2}{3}(\epsilon_1-\epsilon_2)^2$	eqs. (66) and (C.10)	6,1

and (39) may be rewritten as

$$r_{s0}\left(\frac{r_p}{r_s}\right)_2 = \frac{2Q_1(K^2/\epsilon_1\epsilon_2)^2\mathcal{I}_1^2}{(Q_1+Q_2)^3} + \frac{2Q_1Q_2K^2}{(Q_1+Q_2)^2}\,\frac{j_2-(1/\epsilon_1+1/\epsilon_2)i_2}{\epsilon_1-\epsilon_2}. \tag{65}$$

Thus $\mathcal{I}_1$, i_2 and j_2 suffice to characterize s and p reflections to second order. These invariants are given for five simple profiles in table I.

In the evaluation of the invariants it is convenient to position the reference profile to make $\lambda_1 \to 0$ when possible. We then have

$$\begin{aligned} j_2 &= (\epsilon_1-\epsilon_2)J - \left(\frac{1}{\epsilon_1}+\frac{1}{\epsilon_2}\right)\lambda_1\Lambda_1 \\ &\to 2(\epsilon_1-\epsilon_2)^2L^2 \quad (\text{when } \lambda_1 \to 0) \end{aligned} \tag{66}$$

and can use the results of our previous work. Details of invariants not available from published work through (58) and (66) are given in appendix C.

We note in conclusion that the theory developed here, being based on the assumption that ϵ is function of only one spatial coordinate, applies to planar interfaces (of arbitrary profile). Beaglehole[7]) and Zielinska, Bedeaux and Vlieger[8]) have studied reflection from an interface roughened by surface waves. Charmet and de Gennes[10]) have recently developed ellipsometric formulae for films (not necessarily thin) which are bounded by a reflecting wall.

Appendix A

Integral invariants

Let $\epsilon(z)$ be a function with asymptotic values $\epsilon(-\infty)=\epsilon_1$, $\epsilon(+\infty)=\epsilon_2$, and $\epsilon_0(z)$ the step function taking values ϵ_1 for $z<0$ and ϵ_2 for $z>0$. Consider the dependence of

$$\lambda_{n+1}(s) = \int_{-\infty}^{\infty} dz[\epsilon(z-s)-\epsilon_0(z)]z^n \tag{A.1}$$

on the shift parameter s. We have

$$\lambda_{n+1}(s) = \int_{-\infty}^{\infty} dz[\epsilon(z) - \epsilon_0(z) + \epsilon_0(z) - \epsilon_0(z+s)](z+s)^n$$

$$= \int_{-\infty}^{\infty} dz[\epsilon(z) - \epsilon_0(z)](z+s)^n + (\epsilon_1 - \epsilon_2) \int_{-s}^{0} dz(z+s)^n$$

$$= \int_{-\infty}^{\infty} dz[\epsilon(z) - \epsilon_0(z)]\left[z^n + \binom{n}{1} z^{n-1}s + \cdots + s^n\right] + (\epsilon_1 - \epsilon_2)\frac{s^{n+1}}{n+1}$$

$$= \lambda_{n+1}(0) + \binom{n}{1} s\lambda_n(0) + \cdots + s^n\lambda_1(0) + (\epsilon_1 - \epsilon_2)\frac{s^{n+1}}{n+1}. \quad \text{(A.2)}$$

The s-dependence of the first four integrals λ_n is

$$\begin{aligned} \lambda_1(s) &= \lambda_1(0) + (\epsilon_1 - \epsilon_2)s, \\ \lambda_2(s) &= \lambda_2(0) + s\lambda_1(0) + (\epsilon_1 - \epsilon_2)\frac{s^2}{2}, \\ \lambda_3(s) &= \lambda_3(0) + 2s\lambda_2(0) + s^2\lambda_1(0) + (\epsilon_1 - \epsilon_2)\frac{s^3}{3}, \\ \lambda_4(s) &= \lambda_4(0) + 3s\lambda_3(0) + 3s^2\lambda_2(0) + s^3\lambda_1(0) + (\epsilon_1 - \epsilon_2)\frac{s^4}{4}. \end{aligned} \quad \text{(A.3)}$$

We note that

$$2(\epsilon_1 - \epsilon_2)\lambda_2(s) - \lambda_1^2(s) = 2(\epsilon_1 - \epsilon_2)\lambda_2(0) - \lambda_1^2(0) \quad \text{(A.4)}$$

so that

$$i_2 = 2(\epsilon_1 - \epsilon_2)\lambda_2 - \lambda_1^2 \quad \text{(A.5)}$$

is invariant with respect to the relative positioning of ϵ and ϵ_0. Similarly,

$$i_3 = 3(\epsilon_1 - \epsilon_2)^2\lambda_3 - 6(\epsilon_1 - \epsilon_2)\lambda_2\lambda_1 + 2\lambda_1^3 \quad \text{(A.6)}$$

and

$$i_4 = 4(\epsilon_1 - \epsilon_2)^3\lambda_4 - 12(\epsilon_1 - \epsilon_2)^2\lambda_3\lambda_1 + 12(\epsilon_1 - \epsilon_2)\lambda_2\lambda_1^2 - 3\lambda_1^4 \tag{A.7}$$

are invariants. There is an infinite hierarchy of such invariants (assuming the existence of λ_n for all n); the general formula may be obtained from (A.2),

$$i_n = n(\epsilon_1 - \epsilon_2)^{n-1}\lambda_n + \sum_{l=1}^{n-2} (-)^l(n-l)\binom{n}{l}(\epsilon_1 - \epsilon_2)^{n-1-l}\lambda_{n-l}\lambda_1^l + (-)^{n-1}(n-1)\lambda_1^n . \tag{A.8}$$

The invariant i_2 may be expressed as a multiple integral which is manifestly invariant with respect to the location of the profile ϵ relative to the step profile,

$$i_2 = -\int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2[\epsilon(z_1) - \epsilon_0(z_1 - z_2)][\epsilon(z_2) - \epsilon_0(z_2 - z_1)] . \tag{A.9}$$

To verify that (A.9) reduces to (A.5) we use the relations

$$\epsilon_0(z_1 - z_2) - \epsilon_0(z_1) = \begin{cases} \epsilon_2 - \epsilon_1 , & z_2 < z_1 < 0 , \\ \epsilon_1 - \epsilon_2 , & 0 < z_1 < z_2 , \\ 0 , & \text{otherwise} , \end{cases} \tag{A.10}$$

and

$$\int_{-\infty}^{\infty} dz_1[\epsilon_0(z_1 - z_2) - \epsilon_0(z_1)] = (\epsilon_1 - \epsilon_2)z_2 . \tag{A.11}$$

The reciprocal or square of a step function is also a step function; so is any single-valued function of a step function. The invariants developed above thus have endless generalizations. For the physical problem in hand, the invariants arising out of integrals over the difference between the reciprocals of ϵ and ϵ_0 are important. Corresponding to the λ's we define

$$\Lambda_{n+1}(s) = \epsilon_1\epsilon_2 \int_{-\infty}^{\infty} dz\left[\frac{1}{\epsilon_0(z)} - \frac{1}{\epsilon(z-s)}\right]z^n . \tag{A.12}$$

Their transformation properties are the same as those of the λ's: for example

$$\Lambda_1(s) = \Lambda_1(0) + (\epsilon_1 - \epsilon_2)s\,,$$
$$\Lambda_2(s) = \Lambda_2(0) + s\Lambda_1(0) + (\epsilon_1 - \epsilon_2)\frac{s^2}{2}\,. \tag{A.13}$$

Thus

$$I_2 = 2(\epsilon_1 - \epsilon_2)\Lambda_2 - \Lambda_1^2 \tag{A.14}$$

is an invariant, etc. We also have from (A.3) and (A.13) that $\mathscr{I}_1 = \Lambda_1 - \lambda_1$ is an invariant, as is explicitly demonstrated in eq. (11).
The next "mixed" invariant is

$$\begin{aligned}\mathscr{I}_2 &= \epsilon_1\epsilon_2 \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2[\epsilon(z_1) - \epsilon_0(z_1 - z_2)]\left[\frac{1}{\epsilon(z_2)} - \frac{1}{\epsilon_0(z_2 - z_1)}\right] \\ &= (\epsilon_1 - \epsilon_2)(\lambda_2 + \Lambda_2) - \lambda_1\Lambda_1 \\ &= \tfrac{1}{2}(i_2 + I_2 + \mathscr{I}_1^2)\,. \end{aligned} \tag{A.15}$$

Finally, we note that manifestly invariant integrals may be generated by multiplying the integrand in (A.9) by $f(z_1 - z_2)$, where the function f is arbitrary. When $f(z) = e^{ikz}$ we obtain the invariant

$$I(k) = -\int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2\, e^{ik(z_1 - z_2)}[\epsilon(z_1) - \epsilon_0(z_1 - z_2)](\epsilon(z_2) - \epsilon_0(z_2 - z_1))\,. \tag{A.16}$$

On using the relation [cf. (A.11)]

$$\int_{-\infty}^{\infty} dz_1[\epsilon_0(z_1 - z_2) - \epsilon_0(z_1)]\, e^{ikz_1} = \frac{\epsilon_1 - \epsilon_2}{ik}(e^{ikz_2} - 1) \tag{A.17}$$

we find

$$I(k) = \frac{\epsilon_1 - \epsilon_2}{ik}[\lambda(k, s) - \lambda(-k, s)] - \lambda(k, s)\lambda(-k, s)\,, \tag{A.18}$$

where

$$\lambda(k, s) = \int_{-\infty}^{\infty} dz[\epsilon(z-s) - \epsilon_0(z)]\, e^{ikz}$$

$$= e^{iks}\lambda(k, 0) + \frac{\epsilon_1 - \epsilon_2}{ik}(e^{iks} - 1)\,. \tag{A.19}$$

[The second equality in (A.19) may be used to verify that $I(k)$ is an invariant]. We now expand $\lambda(k, s)$ in powers of k. The coefficients are the λ_n integrals defined in (A.1):

$$\lambda(k, s) = \sum_0^{\infty} \frac{(ik)^n}{n!} \lambda_{n+1}(s)\,. \tag{A.20}$$

The invariant $I(k)$ has the expansion

$$I(k) = 2(\epsilon_1 - \epsilon_2) \sum_0^{\infty} \frac{(ik)^{2m}}{(2m+1)!} \lambda_{2m+2} - \sum_0^{\infty}\sum_0^{\infty} \frac{(ik)^n(-ik)^m}{n!m!} \lambda_{n+1}\lambda_{m+1}\,. \tag{A.21}$$

The odd powers of k in (A.21) are zero. The even powers generate a set of invariants which (apart from the first) are distinct from the i_n given earlier: for example the coefficients of $(ik)^2$ and $(ik)^4$ in $I(k)$ are

$$\frac{1}{3}(\epsilon_1 - \epsilon_2)\lambda_4 - \lambda_3\lambda_1 + \lambda_2^2 \tag{A.22}$$

and

$$\frac{1}{60}(\epsilon_1 - \epsilon_2)\lambda_6 - \frac{1}{12}\lambda_5\lambda_1 + \frac{1}{3}\lambda_4\lambda_2 - \frac{1}{4}\lambda_3^2\,. \tag{A.23}$$

The coefficient of $(ik)^0$ is i_2.

Appendix B

Reduction of J and invariance of J_2

The rather complex form of J given in (30) may be simplified as follows.

Consider the double integrals contributing to J; these may be rewritten as

$$\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\int_0^z \frac{d\zeta}{\epsilon}+\int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)\int_0^z d\zeta\epsilon$$

$$=\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\int_0^z d\zeta\left(\frac{1}{\epsilon}-\frac{1}{\epsilon_0}\right)+\int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)\int_0^z d\zeta(\epsilon-\epsilon_0)+\int_{-\infty}^{\infty} dz\, z\left(\frac{\epsilon}{\epsilon_0}-\frac{\epsilon_0}{\epsilon}\right)$$

$$=\frac{\lambda_1^+\Lambda_1-\lambda_1\Lambda_1^+}{\epsilon_1\epsilon_2}+\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\int_z^{\infty} d\zeta\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)$$

$$-\int_{-\infty}^{\infty} dz\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)\int_z^{\infty} d\zeta(\epsilon-\epsilon_0)+\int_{-\infty}^{\infty} dz\, z\left(\frac{\epsilon}{\epsilon_0}-\frac{\epsilon_0}{\epsilon}\right). \tag{B.1}$$

Thus

$$J=2\int_{-\infty}^{\infty} dz\, z\left(\frac{\epsilon}{\epsilon_0}-\frac{\epsilon_0}{\epsilon}\right)+\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\left\{\int_z^{\infty} d\zeta-\int_{-\infty}^{z} d\zeta\right\}\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)$$

$$=2\int_{-\infty}^{\infty} dz\, z\left(\frac{\epsilon}{\epsilon_0}-\frac{\epsilon_0}{\epsilon}\right)+2\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\int_z^{\infty} d\zeta\left(\frac{1}{\epsilon_0}-\frac{1}{\epsilon}\right)-\lambda_1\Lambda_1/\epsilon_1\epsilon_2$$

$$=2\int_{-\infty}^{\infty} dz(\epsilon-\epsilon_0)\left\{\frac{z}{\epsilon}+\int_0^z \frac{d\zeta}{\epsilon(\zeta)}\right\}+\lambda_1(2\Lambda_1^+-\Lambda_1)/\epsilon_1\epsilon_2\,. \tag{B.2}$$

This last form of J verifies (62).

To prove the invariance of J_2 we consider one of a class of manifestly invariant double integrals which are generalizations of $\mathcal{I}_2$ (given by (A.15)):

$$\int_{-\infty}^{\infty} dz_1\int_{-\infty}^{\infty} dz_2 f(z_1-z_2)[\epsilon(z_1)-\epsilon_0(z_1-z_2)]\left[\frac{1}{\epsilon(z_2)}-\frac{1}{\epsilon_0(z_2-z_1)}\right]. \tag{B.3}$$

With $f(z) = \text{sgn}(z)$ this invariant reduces to

$$\int_{-\infty}^{\infty} dz_1[\epsilon(z) - \epsilon_0(z_1)]\left\{\int_{z_1}^{\infty} dz_2 - \int_{-\infty}^{z} dz_2\right\}\left[\frac{1}{\epsilon_0(z_2)} - \frac{1}{\epsilon(z_2)}\right]$$

$$-(\epsilon_1 - \epsilon_2)\int_{-\infty}^{\infty} dz\,|z|\left[\frac{1}{\epsilon_0(z)} - \frac{1}{\epsilon(z)}\right] - \left(\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2}\right)\int_{-\infty}^{\infty} dz\,|z|\,[\epsilon(z) - \epsilon_0(z)]\,. \quad \text{(B.4)}$$

Using the first form for J given in (B.2), and $J_2 = J - (1/\epsilon_1 + 1/\epsilon_2)(\lambda_2 + \Lambda_2)$ we find that the invariant is equal to J_2 plus

$$\int_{-\infty}^{\infty} dz\, z(\epsilon - \epsilon_0)\left\{\frac{1}{\epsilon_1} + \frac{1}{\epsilon_2} + \frac{\epsilon_1 + \epsilon_2}{\epsilon\epsilon_0} - 2\left(\frac{1}{\epsilon_0} + \frac{1}{\epsilon}\right)\right.$$

$$\left. - \frac{\epsilon_1 - \epsilon_2}{\epsilon\epsilon_0}\text{sgn}(z) + \left(\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1}\right)\text{sgn}(z)\right\}. \quad \text{(B.5)}$$

The expressions within the curly brackets in (B.5) is identically zero. We have thus shown that

$$J_2 = \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2\, \text{sgn}(z_1 - z_2)[\epsilon(z_1) - \epsilon_0(z_1 - z_2)]\left[\frac{1}{\epsilon(z_2)} - \frac{1}{\epsilon_0(z_2 - z_1)}\right]. \quad \text{(B.6)}$$

This proves the invariance of J_2, and at the same time demonstrates an unexpected correspondence between J_2 and $\mathcal{J}_2$. Note that from (63), (A.15) and (B.6) we have

$$j_2 = \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \epsilon_0(z_2 - z_1)[\epsilon(z_1) - \epsilon_0(z_1 - z_2)]\left[\frac{1}{\epsilon(z_2)} - \frac{1}{\epsilon_0(z_2 - z_1)}\right]. \quad \text{(B.7)}$$

Appendix C

Definition of profiles, and integrals related to invariants

In the following definitions z_1 is arbitrary, and $z_2 = z_1 + \Delta z$.

Two-step (or uniform layer):

$$\epsilon(z)=\begin{cases}\epsilon_1\,, & z<z_1\,,\\ \epsilon\,, & z_1<z<z_2\,,\\ \epsilon_2\,, & z>z_2\,.\end{cases} \tag{C.1}$$

Linear:

$$\epsilon(z)=\begin{cases}\epsilon_1\,, & z<z_1\,,\\ \epsilon_1+(\epsilon_2-\epsilon_1)(z-z_1)/\Delta z\,, & z_1<z<z_2\,,\\ \epsilon_2\,, & z>z_2\,.\end{cases} \tag{C.2}$$

Rayleigh:

$$\epsilon(z)=\begin{cases}\epsilon_1, & z<z_1,\\ \left[\dfrac{1}{\sqrt{\epsilon_1}}+\left(\dfrac{1}{\sqrt{\epsilon_2}}-\dfrac{1}{\sqrt{\epsilon_1}}\right)(z-z_1)/\Delta z\right]^{-2}, & z_1<z<z_2,\\ \epsilon_2, & z>z_2.\end{cases} \tag{C.3}$$

Exponential:

$$\epsilon(z)=\begin{cases}\epsilon_1+\frac{1}{2}(\epsilon_2-\epsilon_1)\exp(z-z_1)/\Delta z\,, & z<z_1\,,\\ \epsilon_2+\frac{1}{2}(\epsilon_1-\epsilon_2)\exp(z_1-z)/\Delta z\,, & z>z_1\,.\end{cases} \tag{C.4}$$

Hyperbolic tangent, or Fermi function:

$$\begin{aligned}\epsilon(z)&=\tfrac{1}{2}(\epsilon_1+\epsilon_2)-\tfrac{1}{2}(\epsilon_1-\epsilon_2)\tanh[(z-z_1)/2\Delta z]\\ &=\frac{\epsilon_1}{1+\exp(z-z_1)/\Delta z}+\frac{\epsilon_2}{1+\exp(z_1-z)/\Delta z}\\ &=[\epsilon_1+\epsilon_2\exp(z-z_1)/\Delta z]/[1+\exp(z-z_1)/\Delta z]\,.\end{aligned} \tag{C.5}$$

The integrations required for j_2 have been done for the Rayleigh profile[9]), and are elementary for the linear profile. It remains to examine the exponential and Fermi profiles. For those we choose $z_1=0$, which makes $\lambda_1=0$; it then suffices to consider the integral

$$J=2\int_{-\infty}^{\infty}\mathrm{d}z(\epsilon-\epsilon_0)\left\{\frac{z}{\epsilon}+\int_0^z\frac{\mathrm{d}\zeta}{\epsilon(\zeta)}\right\}. \tag{C.6}$$

For the exponential profile

$$\int_0^z \frac{d\zeta}{\epsilon(\zeta)} = \frac{z}{\epsilon_0(z)} + \frac{\Delta z}{\epsilon_0(z)} \operatorname{sgn}(z) \log\left(\frac{2\epsilon(z)}{\epsilon_1 + \epsilon_2}\right). \tag{C.7}$$

For the Fermi profile

$$\int_0^z \frac{d\zeta}{\epsilon(\zeta)} = \frac{z}{\epsilon_1} + \Delta z\left(\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1}\right) \log\left[\frac{\epsilon_1 + \epsilon_2 \exp(z/\Delta z)}{\epsilon_1 + \epsilon_2}\right]$$

$$= \Delta z\left\{\left(\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1}\right)\log\left(\frac{\epsilon(z)}{\epsilon_1 + \epsilon_2}\right) + \frac{1}{\epsilon_2}\log(1 + \exp z/\Delta z)\right.$$

$$\left. - \frac{1}{\epsilon_1}\log(1 + \exp(-z/\Delta z))\right\}. \tag{C.8}$$

The J integral may be further reduced by elementary manipulations. For the exponential profile we find

$$J = 2(\Delta z)^2\left\{\log\frac{\epsilon_1}{\epsilon_2} + \int_{(\epsilon_2-\epsilon_1)/2\epsilon_1}^{(\epsilon_1-\epsilon_2)/2\epsilon_2} dx\, \frac{\log(1+x)}{x}\right\}. \tag{C.9}$$

The leading term in an expansion in terms of $\delta = (\epsilon_1 - \epsilon_2)/(\epsilon_1 + \epsilon_2)$ is $8(\Delta z)^2\delta$. For the Fermi profile there is a large number of equivalent analytical forms. We give one which is convenient for numerical computation:

$$J = 2(\Delta z)^2(\epsilon_1 - \epsilon_2)\left\{\frac{\pi^2}{6}\left(\frac{1}{\epsilon_1} + \frac{1}{\epsilon_2}\right)\right.$$

$$\left. + \frac{\epsilon_1 - \epsilon_2}{\epsilon_1\epsilon_2}\int_0^1 \frac{dx}{1+x}\left[\log\left(\frac{\epsilon_1 x + \epsilon_2}{\epsilon_1 + \epsilon_2 x}\right) + \frac{(\epsilon_1^2 - \epsilon_2^2)x \log x}{(\epsilon_1 x + \epsilon_2)(\epsilon_1 + \epsilon_2 x)}\right]\right\}. \tag{C.10}$$

The leading term in the δ expansion is $(4\pi^2/3)(\Delta z)^2\delta$.

References

1) J. Lekner, Physica **112A** (1982) 544, referred to here as I.
[Some aspects of s-wave reflection were previously treated by D.G. Triezenberg in his thesis (University of Maryland (1973), unpublished).]
2) J. Lekner, Physica **113A** (1982) 506, referred to here as II.
3) P. Drude, The Theory of Optics (Dover, London, 1959), pp. 287–295.
4) L. Lorenz, Pogg. Ann. **111** (1980) 460.
5) J.W.S. Rayleigh, Proc. Roy. Soc. **86** (1912) 207.
6) J. Lekner, Mol. Phys. **49** (1983) 1385.
7) D. Beaglehole, Physica **100B** (1980) 163.
8) B.J.A. Zielinska, D. Bedeaux and J. Vlieger, Physica **107A** (1981) 91, **117A** (1983) 26.
9) J. Lekner, Physica **116A** (1982) 235.
10) J.C. Charmet and P.G. de Gennes, to be published.