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Reflection of waves by a profile with discontinuities

John Lekner

Department of Physics, Victoria University of Wellington, Wellington, New Zealand

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Abstract. Formulae are derived for the reflection and transmission amplitudes for a potential or dielectric function profile which has discontinuities in value and/or slope at its boundaries. These formulae, which are based on the Liouville-Green wavefunctions, are accurate at short wavelengths in general, and exact at all wavelengths for the uniform layer. A comparison with an exactly solvable model profile is made.

1. Introduction

In the propagation of electromagnetic, acoustic, or particle waves in stratified media, the reflection or transmission by a planar stratification is given by the absolute square of the reflection and transmission amplitudes r and t, defined by

$$e^{iq_1z} + r\,e^{-iq_1z} \leftarrow \psi(z) \rightarrow t\,e^{iq_2z}. \tag{1}$$

In some cases (ellipsometry, reflection of beams or pulses), the phase of the complex quantities r and t is important, so we will retain phase information here. The total wavefunction, for plane waves propagating in the z-x plane, in a medium whose properties depend on the z coordinate only, is

$$\Psi(x, z) = \exp(iKx)\psi(z) \tag{2}$$

where K is the x component of the wavevector, and $\psi(z)$ satisfies

$$\frac{d^2\psi}{dz^2} + q^2(z)\psi = 0. \tag{3}$$

The normal or z component of the wavevector is given, for the electromagnetic s wave and for particle waves, by

$$q^2(z) = \varepsilon(z)\frac{\omega^2}{c^2} - K^2 \qquad q^2(z) = \frac{2m}{\hbar^2}(E - V(z)) - K^2. \tag{4}$$

Here $\varepsilon(z)$ is the dielectric function, ω is the angular frequency of the electromagnetic wave, c is the speed of light; m, E and $V(z)$ are the mass, total energy and potential energy of the particle. The electromagnetic p wave and acoustic waves satisfy equations a little more complicated than (3) (see Lekner 1987, sections 1.2 and 1.4), but similar techniques to those developed here can be used.

A general-purpose formula for the reflection amplitude is the Rayleigh or weak-reflection approximation

$$r_R = -\int_{-\infty}^{\infty} \mathrm{d}z \frac{q'}{2q} \exp 2\mathrm{i}\phi \tag{5}$$

where ϕ is the phase integral

$$\phi(z) = \int^{z} \mathrm{d}z\, q(\zeta) \tag{6}$$

(the lower limit in (6) is to be chosen so as to make $\phi \to q_1 z$ as $z \to -\infty$; see Lekner (1987, section 5.6)). This approximation goes back to Rayleigh (1912) and can be derived from the Bremmer (1949, 1951) method; see Berry and Mount (1972, section 2.3, equation (2.29)). The derivation of (5) from a Riccati equation in Lekner (1987), section 5.7, shows directly that it applies only if the reflection is weak; hence the alternative name *weak reflection approximation.* The Rayleigh approximation works very well when the reflection is small (see Lekner 1987, figures 5.4 and 6.3), but for the case considered here, with discontinuities in $\varepsilon(z)$ or $V(z)$, the reflection can be strong, even in the short-wave limit. As an example, consider the step profile, where $\varepsilon(z)$ or $V(z)$ change discontinuously at $z=0$: the reflection amplitude is

$$r_{\text{step}} = \frac{q_1 - q_2}{q_1 + q_2} \tag{7}$$

which is independent of frequency in the electromagnetic case. The Rayleigh approximation (5) gives $\frac{1}{2}\log(q_1/q_2)$ in this case, which is close to (7) only when $q_1/q_2 - 1$ is small, and fails completely for small or large values of the ratio q_1/q_2.

In this paper we will develop a method for calculating the reflection amplitude which is accurate in the case of discontinuities in ε or V, and thus can replace the Rayleigh approximation. For concreteness and in order to provide an explicit formula, we will restrict ourselves to the case where the discontinuities occur at the boundaries of the stratification, as for example in figure 1.

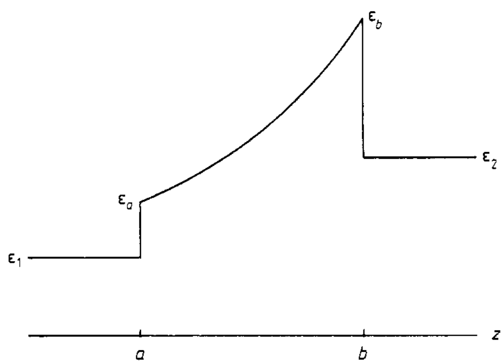

Figure 1. A dielectric function profile representing a stratified planar inhomogeneity between $z=a$ and $z=b$. The profile shown has the reciprocal of the refractive index linear in z (see equation (20) in section 3). The values used are $\varepsilon_1 = 1$, $\varepsilon_a = (1.3)^2$, $\varepsilon_b = 4$, and $\varepsilon_2 = (1.5)^2$, representing a dielectric layer between air and glass, at optical frequencies.

2. Formulae for *r* and *t* based on Liouville–Green wavefunctions

In this section we will use the general formulae (2.25) and (2.26) of Lekner (1987), together with the Liouville (1837) and Green (1837) approximate solutions of (3), namely

$$\psi_+ = \left(\frac{q_a}{q}\right)^{1/2} \exp(\mathrm{i}\phi) \qquad \psi_- = \left(\frac{q_b}{q}\right)^{1/2} \exp(-\mathrm{i}\phi). \tag{8}$$

These approximate solutions, also known as the WKB or JWKB wavefunctions, are discussed in more detail in Lekner (1987, section 6.2). The general formulae referred to above are

$$r = \mathrm{e}^{2\mathrm{i}\alpha} \frac{q_1q_2(F, G) + \mathrm{i}q_1(F, G') + \mathrm{i}q_2(F', G) - (F', G')}{q_1q_2(F, G) + \mathrm{i}q_1(F, G') - \mathrm{i}q_2(F', G) + (F', G')} \tag{9}$$

$$t = \mathrm{e}^{\mathrm{i}(\alpha - \beta)} \frac{2\mathrm{i}q_1(F_bG'_b - G_bF'_b)}{q_1q_2(F, G) + \mathrm{i}q_1(F, G') - \mathrm{i}q_2(F', G) + (F', G')} \tag{10}$$

where $\alpha = q_1a$, $\beta = q_2b$, F and G are two independent solutions of (3), and

$$(F, G) \equiv F_aG_b - G_aF_b \qquad (F, G') \equiv F_aG'_b - G_aF'_b \tag{11}$$

etc. Here F_a stands for $F(z)$ evaluated at $z = a$, F'_a for the derivative of $F(z)$ evaluated at $z = a$, and so on. Since q is discontinuous at a and b, and (8) are valid approximations only for $a < z < b$, the values and derivatives at a and b are to be understood as limits $z \searrow a$ and $z \nearrow b$, respectively.

The formulae (9) and (10) are exact, but in general analytic solutions of (3) are not available. Our approximation consists in replacing F by ψ_- and G by ψ_+. The resulting approximate values of (F, G) to (F', G') are then

$$\begin{aligned}
(F, G) &\approx -2\mathrm{i} \sin \Delta\phi \\
(F, G') &\approx \mathrm{i}q_b(-2 \cos \Delta\phi + \gamma_b \sin \Delta\phi) \\
(F', G) &\approx \mathrm{i}q_a(2 \cos \Delta\phi + \gamma_a \sin \Delta\phi) \\
(F', G') &\approx \mathrm{i}q_aq_b(-2 \sin \Delta\phi + (\gamma_a - \gamma_b) \cos \Delta\phi - \tfrac{1}{2}\gamma_a\gamma_b \sin \Delta\phi).
\end{aligned} \tag{12}$$

The quantities γ_a and γ_b are values at $z = a$ and b of the dimensionless function $\gamma = q'/q^2$ (which should be small in order for $\psi_\pm$ to be accurate solutions of (3); see Lekner (1987, section 6.2)), and

$$\Delta\phi \equiv \phi(b) - \phi(a) = \int_a^b \mathrm{d}z\, q(z) \tag{13}$$

is the phase increment on going through the stratification from a to b. The Wronskian $FG' - GF'$ in the numerator of (10) is independent of z, and when F, G are approximated by ψ_+, ψ_- takes the value $-2\mathrm{i}(q_aq_b)^{1/2}$. Since the approximation relies on γ_a and γ_b being small, we shall keep only terms of first order in γ_a and γ_b in evaluating r and t. The results are, with c and s standing for the cosine and sine of $\Delta\phi$,

$$r = r_0 + r_1 + \ldots \qquad t = t_0 + t_1 + \ldots \tag{14}$$

where

$$r_0 = e^{2i\alpha} \frac{(q_1 q_b - q_2 q_a)c + (q_a q_b - q_1 q_2)\, is}{(q_1 q_b + q_2 q_a)c - (q_a q_b + q_1 q_2)\, is} \tag{15}$$

$$r_1 = e^{2i\alpha} \frac{iq_1 q_a \{q_b^2(\gamma_b - \gamma_a)c^2 + (q_b^2\gamma_b + q_2^2\gamma_a)s^2 + 2iq_b q_2 \gamma_a cs\}}{[(q_1 q_b + q_2 q_a)c - (q_a q_b + q_1 q_2)\, is]^2}. \tag{16}$$

When $q_a = q_b$ (15) reduces to the uniform layer reflection amplitude (see for example Lekner (1987), equation (2.52)). When $q_a = q_1$ and $q_b = q_2$, that is when there is no discontinuity in ε or V at either $z = a$ or $z = b$, (15) is zero and (16) reduces to equation (6.35) of Lekner (1987).

The corresponding results for the transmission amplitude are

$$t_0 = e^{i(\alpha-\beta)} \frac{2q_1(q_a q_b)^{1/2}}{[(q_1 q_b + q_a q_2)c - (q_a q_b + q_1 q_2)\, is]} \tag{17}$$

$$t_1 = e^{i(\alpha-\beta)} \frac{q_1(q_a q_b)^{1/2}[(q_1 q_b \gamma_b - q_a q_2 \gamma_a)s - q_a q_b(\gamma_a - \gamma_b)\, ic]}{[(q_1 q_b + q_a q_2)c - (q_a q_b + q_1 q_2)\, is]^2}. \tag{18}$$

When $q_a = q_b$ (17) reduces to the uniform layer transmission amplitude (Lekner 1987, equation 2.53). In the continuous profile case ($q_a = q_1$, $q_b = q_2$), t_0 takes the perfect transmission value $e^{i(\alpha-\beta)}(q_1/q_2)^{1/2} e^{i\Delta\phi}$, and

$$t_1 = e^{i(\alpha-\beta)} \left(\frac{q_1}{q_2}\right)^{1/2} e^{i\Delta\phi} \frac{i}{4}(\gamma_b - \gamma_a). \tag{19}$$

These expressions are the zeroth and first-order parts of $t^{(1)}$ given in Lekner (1987, equation (6.46)).

The expressions (15)-(18) are high-frequency approximations for the reflection and transmission amplitudes due to a profile with arbitrary discontinuities, in value and in slope, at its boundaries. In the next section the reflectivity deduced from (15) and (16) is compared with the exact reflectivity of a solvable model profile.

3. A solvable discontinuous model profile

The results of the previous section have been seen to reproduce the exact r and t for a uniform layer (a discontinuous profile with constant value of ε or V over its extent). To test the formulae derived there in the more general case of variable ε or V, we will generalise a model continuous profile introduced by Rayleigh (1880). In optical terms, the Rayleigh profile is one in which the reciprocal of the refractive index varies linearly with displacement normal to the interface. We thus set (cf Lekner 1982)

$$\varepsilon^{-1/2}(z) \equiv \eta(z) = \eta_a + (z-a)\frac{\Delta\eta}{\Delta z} \tag{20}$$

where $\eta_a = \varepsilon_a^{-1/2}$, $\eta_b = \varepsilon_b^{-1/2}$, $\Delta\eta = \eta_b - \eta_a$, $\Delta z = b - a$. On changing the independent variable in (3) from z to η, we have (at normal incidence)

$$\frac{d^2\psi}{d\eta^2} + \left(\frac{1}{4} - \nu^2\right)\frac{\psi}{\eta^2} = 0 \qquad \nu^2 = \frac{1}{4} - \left(\frac{\omega}{c}\frac{\Delta z}{\Delta\eta}\right)^2. \tag{21}$$

The solutions for ψ are $\eta^{(1/2)\pm\nu}$ (at arbitrary angle of incidence the solutions are Bessel functions; see Lekner (1982)). We can thus set $F=\eta^{(1/2)+\nu}$, $G=\eta^{(1/2)-\nu}$ and use the general formulae (9) and (10). To simplify the resulting expressions, we use the conventional optical notation of n for refractive index ($n=\varepsilon^{1/2}=\eta^{-1}$), with μ equal to the ratio of the refractive indices,

$$\mu=\frac{n_b}{n_a}=\left(\frac{\varepsilon_b}{\varepsilon_a}\right)^{1/2}=\frac{\eta_a}{\eta_b}. \tag{22}$$

We find

$$\begin{aligned}
(F,G)&=(n_a n_b)^{-1/2}(\mu^{\nu}-\mu^{-\nu})\\
(F,G')&=\frac{\Delta\eta}{\Delta z}\mu^{1/2}[\tfrac{1}{2}(\mu^{\nu}-\mu^{-\nu})-\nu(\mu^{\nu}+\mu^{-\nu})]\\
(F',G)&=\frac{\Delta\eta}{\Delta z}\mu^{-1/2}[\tfrac{1}{2}(\mu^{\nu}-\mu^{-\nu})+\nu(\mu^{\nu}+\mu^{-\nu})]\\
(F',G')&=\frac{\omega^2}{c^2}(n_a n_b)^{1/2}(\mu^{\nu}-\mu^{-\nu}).
\end{aligned} \tag{23}$$

Let us write μ^{ν} as e^{θ}, where $\theta=\nu\log\mu$. With this substitution in (23), (9) and (10) give

$$r=e^{2i\alpha}\frac{2(n_1n_2-n_an_b)\sinh\theta+i(c/\omega)(\Delta\eta/\Delta z)\times[n_1n_b(\sinh\theta-2\nu\cosh\theta)+n_2n_a(\sinh\theta+2\nu\cosh\theta)]}{2(n_1n_2+n_an_b)\sinh\theta+i(c/\omega)(\Delta\eta/\Delta z)\times[n_1n_b(\sinh\theta-2\nu\cosh\theta)-n_2n_a(\sinh\theta+2\nu\cosh\theta)]} \tag{24}$$

$$t=e^{i(\alpha-\beta)}\frac{-4in_1(n_an_b)^{1/2}\nu(c/\omega)(\Delta\eta/\Delta z)}{2(n_1n_2+n_an_b)\sinh\theta+i(c/\omega)(\Delta\eta/\Delta z)\times[n_1n_b(\sinh\theta-2\nu\cosh\theta)-n_2n_a(\sinh\theta+2\nu\cosh\theta)]}. \tag{25}$$

When $n_a=n_1$ and $n_b=n_2$ (no discontinuity in dielectric function at $z=a$ or b), these expressions reduce to

$$r=e^{2i\alpha}\frac{-\frac{1}{2}\sinh\theta}{\nu\cosh\theta+i(\omega/c)(\Delta z/\Delta\eta)\sinh\theta} \tag{26}$$

$$t=e^{i(\alpha-\beta)}\frac{\nu(n_1/n_2)^{1/2}}{\nu\cosh\theta+i(\omega/c)(\Delta z/\Delta\eta)\sinh\theta}. \tag{27}$$

The first of these is in agreement with equation (9) of Lekner (1982).

The analytic form of all of these expressions changes when the magnitude of the dimensionless quantity $f=(\omega/c)(\Delta z/\Delta\eta)$ passes through the value $\frac{1}{2}$. When $|f|>\frac{1}{2}$, ν becomes imaginary: $\nu=i|\nu|$. The reflection and transmission amplitudes in this case are obtained from (24) and (25) by the substitutions

$$\cosh\theta\to\cos|\theta| \qquad \sinh\theta\to i\sin|\theta|. \tag{28}$$

The high-frequency limiting forms of r and t are obtained in this way, making use of the fact that when $|f|$ is large, $\nu\to i|f|$. We find

$$r\to e^{2i\alpha}\frac{(n_1n_b-n_2n_a)\cos\Delta\phi+i(n_an_b-n_1n_2)\sin\Delta\phi}{(n_1n_b+n_2n_a)\cos\Delta\phi-i(n_an_b+n_1n_2)\sin\Delta\phi} \tag{29}$$

$$t\to e^{i(\alpha-\beta)}\frac{2n_1(n_an_b)^{1/2}}{(n_1n_b+n_2n_a)\cos\Delta\phi-i(n_an_b+n_1n_2)\sin\Delta\phi}. \tag{30}$$

Here we have used the phase increment for the Rayleigh profile,

$$\Delta\phi = -\frac{\omega}{c}\frac{\Delta z}{\Delta\eta}\log\mu = -f\log\mu. \tag{31}$$

These expressions are in exact concord with the normal-incidence versions of (15) and (17).

4. Comparison of theory with the solvable model, and discussion

We have already noted that the theory based on the Liouville–Green approximate wavefunctions is asymptotically correct in the high-frequency limit, for a particular solvable model. How well does the theory work at intermediate frequencies? Figure 2 shows the normal-incidence reflectivity as a function of the dimensionless parameter $\omega\Delta z/c$. The refractive indices chosen for the comparison are $n_1 = 1$, $n_a = 1.3$ $n_b = 2$, $n_2 = 1.5$, corresponding to an inhomogeneous dielectric layer between air and glass. (The corresponding dielectric function, assuming a Rayleigh profile for the transition, was shown in figure 1.) The theoretical expressions (15) and (16) require $\Delta\phi$, given in (31), and the parameters γ_a and γ_b. For the Rayleigh profile at normal incidence, these are equal since then $\gamma = q'/q^2$ reduces to

$$\gamma = \frac{n'}{(\omega/c)n^2} = -\left(\frac{\omega}{c}\frac{\Delta z}{\Delta\eta}\right)^{-1} \equiv -f^{-1}. \tag{32}$$

The resulting r_0 is the same as (20), as noted before, and the resulting r_1 is, with c and s again standing for cosine and sine of $\Delta\phi$,

$$r_1 = \frac{(n_1 n_a s/f)[2n_b n_2 c - \mathrm{i}(n_b^2 + n_2^2)s]}{[(n_1 n_b + n_2 n_a)c - \mathrm{i}(n_a n_b + n_1 n_2)s]^2}. \tag{33}$$

The agreement between the theory based on the Liouville–Green wavefunctions and the exact solution is seen to be good. At low frequency it is better than can be expected in general: it is a special feature of the Rayleigh profile that $\gamma_a = \gamma_b$ (at normal

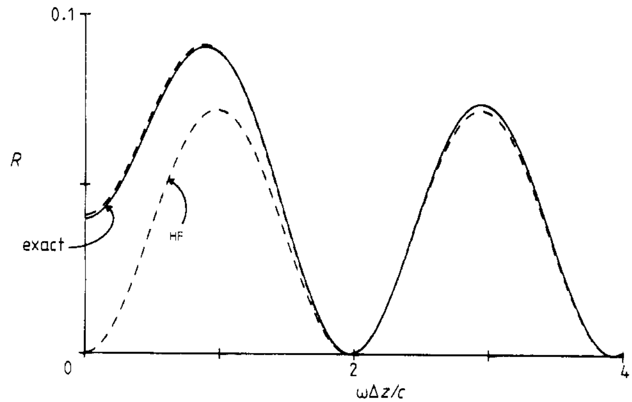

Figure 2. Exact and approximate normal incidence reflectivities for the dielectric function profile shown in figure 1. The full curve is the exact reflectivity, obtained as the absolute square of (24). The two broken curves are the high-frequency limiting form $|r_0|^2$, given by (29), and $|r_0 + r_1|^2$, with r_1 given by (33).

incidence only). This removes the divergent term proportional to $(\gamma_a - \gamma_b)\cos^2\Delta\phi$ in (16). (The divergence of γ at zero frequency can be seen in the first equality of (32).) Thus in general the theory will fail at low frequencies, as can be expected from the nature of the Liouville–Green approximation to the wavefunctions (see Lekner 1987, section 6.2). The low-frequency end of the spectrum has been determined for arbitrary profiles (Lekner 1984 and Lekner 1987, chapter 3); for the electromagnetic s wave and for particle waves the reflectivity is given by

$$R = |r_{\text{step}}|^2 - \frac{4q_1q_2(\omega/c)^4}{(q_1+q_2)^4}\, i_2 + \ldots \tag{34}$$

where i_2 is an integral invariant, a characteristic of a given profile. The general form of i_2 is given in the references just quoted. From this we find, for the discontinuous Rayleigh profile,

$$i_2 = (\Delta z)^2\left(\frac{(\varepsilon_1-\varepsilon_2)\varepsilon_a\varepsilon_b}{(\sqrt{\varepsilon_a}-\sqrt{\varepsilon_b})^2}\log\frac{\varepsilon_a}{\varepsilon_b} - \varepsilon_a\varepsilon_b - \varepsilon_1\varepsilon_2 - 2\frac{\sqrt{\varepsilon_a\varepsilon_b}}{\sqrt{\varepsilon_a}-\sqrt{\varepsilon_b}}(\varepsilon_1\sqrt{\varepsilon_b}-\varepsilon_2\sqrt{\varepsilon_a})\right). \tag{35}$$

The low-frequency reflectivity given by (34) and (35) is shown in figure 3, together with the exact and approximate reflectivities shown before in figure 2.

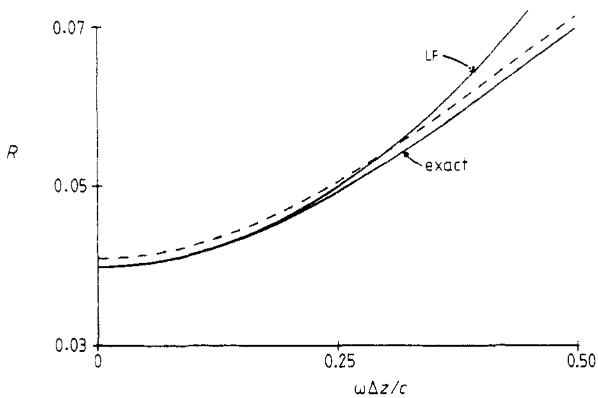

Figure 3. Detail of the low-frequency reflectivity for the Rayleigh profile at normal incidence. The profile parameters are as in figures 1 and 2. The low-frequency limiting form, given by (34) and (35), is labelled LF.

We remark finally on the *periodicity* (in the limit of high frequencies) of the exact and approximate reflectivities in the frequency–thickness parameter $\omega\Delta z/c$. This is due to the discontinuities in the profile. Actual dielectric functions or potential energies may change rapidly, but will not change discontinuously, and thus actual reflectivities will eventually (at high enough frequencies or energies) lose periodicity and decay to zero when the changes in ε or V no longer appear suddenly on the scale of the wavelength.

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