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Reflection coefficient due to a discontinuity in the *n*th order derivative of the refractive index

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Abstract

Surfaces within a dielectric material, where the derivatives of a continuous and real refractive index profile are discontinuous, are shown to enhance reflection. To this end, the amplitude and phase representation of electromagnetic waves is used to model light propagating normally through a transparent medium with a continuous refractive index profile that varies only in one spatial direction. The amplitude equation is solved under the slowly varying refractive index approximation (SVRI). To isolate the effect of a single surface where the refractive index derivatives are discontinuous, an $n(z)$ profile is proposed that is analytical, smooth and slowly varying except for a single piecewise junction. At this junction, $n(z)$ is continuous but some of the mth order derivatives are not. Two different SVRI approximated solutions are joined at the discontinuity plane and, by demanding that boundary conditions are satisfied, a general complex reflection coefficient is obtained. By categorizing profiles according to the lowest order discontinuous derivative at the junction, a simple expression for the reflection coefficient can be written. Results are compared favorably with previous numerical solutions. Furthermore, a conjecture by the authors in a previous paper, 'for a C^{m-1} refractive index profile type, where m stands as the order of the lowest order discontinuous derivative, phase change upon reflection at the discontinuity plane is $(2-m)\frac{\pi}{2}$ for an increasing lowest order discontinuous derivative and $-m\frac{\pi}{2}$ for the decreasing case', is proved here.

Keywords: electromagnetic wave propagation, stratified media, reflectivity, discontinuity, rugate filters, optical coatings, optical coherence tomography
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(Some figures may appear in colour only in the online journal)

1. Introduction

The reflectivity produced by changes in the refractive index has been studied at least since Fresnel days. The abrupt limit between two dielectrics or the very slowly varying refractive index approximation are quite tractable, leading to Fresnel relationships or a null reflectivity respectively. Variations of the refractive index on the wavelength scale produce reflectivities from the bulk that are much more difficult to handle. Reflectivities arising from derivatives of the refractive index have hardly been treated. Furthermore, mostly isolated cases have been undertaken. Nonetheless, precise reflectivity calculations are needed, particularly now that various imaging methods, such as optical coherence tomography, rely on the reflection of light in order to reconstruct the object optical properties.

In recent papers, a method to find numerical solutions for the electric field equation by solving the associated amplitude equation was proposed [1–3]. After solving the amplitude equation for numerous $n(z)$ profiles, with different types of derivative discontinuity, a consistent behavior was found [1]. When $n(z)$ varies slowly enough that the significant source of reflection is a discontinuity in the mth order derivative, the complex reflection coefficient depends mainly on m and the difference between the value of this derivative on both sides of the discontinuity $\Delta(\mathrm{d}^m n/\mathrm{d}z^m)$, regardless of the profile particular functional form. Computed reflectivity diminishes for a greater m and a smaller values of $\Delta(\mathrm{d}^m n/\mathrm{d}z^m)$. For the phase relationship between incident and reflected waves, every case seems to follow approximately the same rule: 'for a C^{m-1} refractive index profile type, where m stands as the order of the lowest order discontinuous derivative, phase change upon reflection at the discontinuity plane is $(2-m)\frac{\pi}{2}$ for an increasing lowest order discontinuous derivative and $-m\frac{\pi}{2}$ for the decreasing case'. The purpose of the present work is to provide a formal proof. We view this behavior as a generalization of the Fresnel result, for normal incidence, to include the case of discontinuous derivatives, not only discontinuities in $n(z)$ itself.

In this paper, the complex reflection coefficient at normal incidence is derived for very general refractive index discontinuities, not for a discontinuous $n(z)$, a case which is very well known, but for discontinuous derivatives $\frac{\mathrm{d}^m n}{\mathrm{d}z^m}$. From the modulus, the ratio of the incident to reflected amplitudes is obtained at an arbitrary dielectric discontinuity. From the argument, the phase change upon reflection is obtained, thus proving the proposition stated by the authors in a previous paper [1]. To seek our analytical proof we employ the so called JWKB (or simply WKB) approximation. This approximation is typically used in quantum mechanics to solve the time independent Schrödinger equation, when the length scale over which the potential changes is large compared to the de Broglie wavelength. In fact, it is a general method to solve approximately differential equations with spatially varying coefficients [4]. Although it was developed fully between 1923 and 1926, earlier references to the method include a Rayleigh paper where it is applied to optics and stratified media [5]. In a recent paper [6], it was shown that the Ermakov equation can be solved under the JWKB approximation, if provided with a small parameter as a factor of the second derivative term. In our case, the JWKB approximation is physically equivalent to a 'slowly varying refractive index approximation' (SVRI); the length scale over which the refractive index changes is large compared to the wavelength.

The structure of this manuscript is as follows: we start by summarizing previous reflection coefficient results for continuous refractive index profiles in one dimension. The case when this coefficient is related to discontinuities in the derivatives of a continuous refractive index profile is emphasized. In section 2, we propose that the amplitude equation, being an Ermakov–Milne–Pinney type equation, can be solved under the SVRI approximation; this solution is expressed as a series expansion in powers of k_0^{-2}. Each order j of the expansion is a set of terms that involve all $\frac{\mathrm{d}^m n}{\mathrm{d}z^m}$ derivatives up to the jth order. In the next sections, from 3 to 5, we present our main original proposal. In section 3 we demonstrate that, from the set of terms corresponding to the jth order in the expansion, the single term with the highest order derivative $\frac{\mathrm{d}^j n}{\mathrm{d}z^j}$ can always be written explicitly in a simple way. Although the SVRI solution proposed in section 2 is a particular solution, it is shown in section 4 that a more general solution can be devised based on the superposition principle, one that allows counter-propagation. By piecewise joining two different SVRI solutions and demanding that the field boundary conditions are satisfied, a reflection coefficient is obtained for the junction plane. This reflection coefficient turns out to be a quotient written in terms of the squared amplitude equation solutions and their derivatives. By classifying the profiles $n(z)$ according to their lowest order discontinuous derivative at the junction and using the highest order derivative term found in section 3, we write explicit and simple expressions for the reflection coefficient to leading order in the SVRI approximation in section 5. In sections 6–8, comparisons between our novel results and those recalled in section 2 are established. Reflection enhancement is confirmed when the reflectivity for analytic profiles is examined in contrast with the one for piecewise profiles that have a junction plane, where the refractive index derivatives are discontinuous. Previous numerical results are compared with the present approximate analytic ones. A couple of examples of known reflection coefficients are shown to be consistent with the derivation proposed in this work. Some applications are suggested. Finally, conclusions in section 9 summarize the main results and place the proposition regarding the phase change upon reflection at an arbitrary dielectric discontinuity on a firm ground.

1.1. Previous reflection coefficient results

The electric field equation for plane monochromatic waves has been solved in closed form for different refractive index continuous profiles $n(z)$, with or without approximations [7, Chapter III]. Epstein solved it exactly in [8], using a fully analytic refractive index profile that accurately models a transitional interface, smoothly and monotonically changing from n_1 to n_2. In the same article Epstein also found a solution for a symmetrical profile, resembling a standing thin film that evolves from n_1 to n_3 and back to n_1. These profiles are now called 'Epstein layers':

$$n_{\text{trans}}^2(z) = \frac{n_1^2+n_2^2}{2} + \frac{n_2^2-n_1^2}{2}\tanh\left(\frac{k_0}{2s}z\right)$$
$$\text{and} \qquad n_{\text{sym}}^2(z) = n_1^2 + \frac{n_3^2}{4\cosh^2(\frac{k_0}{2s}z)}, \tag{1}$$

where s is a parameter proportional to the interface or film thickness. Both solutions were obtained in terms of hypergeometric series. An explicit and notably simple result for the reflectivity of the first one was yielded:

$$R = \frac{\sinh^2[\pi s(n_2-n_1)]}{\sinh^2[\pi s(n_2+n_1)]}. \tag{2}$$

In the abrupt limit, for $s \to 0$, Fresnel relation $R = (n_2-n_1)^2/(n_2+n_1)^2$ is recovered, while for the slowly varying case, as $s \to \infty$, the reflectivity asymptotically tends to zero. Somehow, Epstein did not pay attention to the complex reflection coefficient and its phase. Later, Brekhovskikh [7], in a thorough review of important exact solutions for the electric field equation with a continuous $n(z)$, writes this coefficient explicitly.

In early works [5, 9], the reflection coefficient for a continuous function $n(z)$, with a linear behavior in the propagation speed, bounded by one or two homogeneous media was presented. This Rayleigh profile involves one or two piecewise junctions, where the derivative $\mathrm{d}n/\mathrm{d}z$ is discontinuous, changing from zero to another real value. The Rayleigh profile with a single junction, for normal incidence, can be written as [7]

$$n(z) = \begin{cases} \dfrac{a}{d} & z \le 0 \\ \dfrac{a}{(z+d)} & z > 0 \end{cases} \tag{3}$$

and its reflection coefficient as

$$r = \frac{1 - \frac{1}{2\mathrm{i}k_0 a} - \sqrt{1 - \frac{1}{4k_0^2 a^2}}}{1 + \frac{1}{2\mathrm{i}k_0 a} + \sqrt{1 - \frac{1}{4k_0^2 a^2}}}, \tag{4}$$

where a and d are real constants. Brekhovskikh and Jacobsson [10] later reviewed his results, comparing them with Epstein's. They pointed out that, in the two junction case, the reflectivity oscillates and presents interference nulls.

Another interesting profile with an exact analytic solution is

$$n^2(z) = \begin{cases} 1 & z \le 0 \\ 1 + az & z > 0 \end{cases}, \tag{5}$$

where a is a real constant [11]. It has one piecewise junction between a homogeneous medium and an inhomogeneous half space, introducing a discontinuity in the refractive index first derivative. The reflection coefficient r, reported for small positive values of a/k_0, that is, for a slowly varying refractive index, is [7]

$$r = -\frac{\mathrm{i}a}{8k_0 \cos^3\theta_0}. \tag{6}$$

There are other closed form solutions of the electric field equation, with continuous and explicit profiles $n(z)$; most are well reviewed in [7]. Whenever they involve piecewise junctions in their profiles, they are always homogeneous to inhomogeneous media transitions.

The reflection coefficient has also been obtained from approximate solutions. Kofink and Menzer [12] modeled a thin film on a substrate; an inhomogeneous region was bounded at each side by homogeneous media with constant refractive indices n_i and n_t. While the profile could only be discontinuous at the borders, the inhomogeneous part could change quite arbitrarily, but smoothly enough for the JWKB approximation to be valid. Performing a change of variable on the linear electric field equation for the inhomogeneous region, a Riccati equation was obtained. The JWKB approximation was invoked to solve it. Boundary conditions were adjusted by piecewise joining with the homogeneous region's solutions. Even if the whole $n(z)$ profile was gradual and continuous, the two junctions worked as reflection planes due to discontinuous jth order derivatives of the refractive index. It was clear that these derivative discontinuities enhanced reflection. A rough relation was noticed between overall reflectivity and the type of derivative discontinuity at the borders. Reflectivity was evaluated for the complete three region medium, not for each particular junction, neither was attention paid to the phase relationship between the counter-propagating waves. A rough relation was noticed between overall reflectivity and the type of derivative discontinuity. If the jth derivative changes discontinuously but all lower derivatives are continuous, as well as $n(z)$ itself, then $R \sim (1/k_0 d)^{2j}$, where d is the thin film thickness [10, 12].

2. The amplitude equation under the SVRI approximation

Consider Maxwell's equations, in an isotropic, transparent, dielectric medium with a linear response and no free charges, let the electric permittivity and magnetic permeability vary spatially in the direction of stratification, so that ϵ and μ will depend only on z. Under these conditions, for a monochromatic plane wave with frequency ω and linear TE polarization, say, in the x direction $\mathbf{E} = E(y, z)\mathrm{e}^{-\mathrm{i}\omega t}\,\hat{\mathbf{e}}_x$, a partial differential equation (PDE) for the electric field is obtained [13, equation (3), section 1.6.1, p 55]. For normal incidence and non-magnetic media $\mu = \mu_0$, this PDE becomes the non-autonomous ordinary differential equation (ODE)

$$\frac{\mathrm{d}^2E}{\mathrm{d}z^2} + k_0^2 n^2 E = 0, \tag{7}$$

where $k_0^2 = \omega^2\mu_0\varepsilon_0$ and the refractive index is $n = \sqrt{\frac{\varepsilon(z)}{\varepsilon_0}}$; ε_0 is the electric permittivity of vacuum. This ODE is the electric field equation for plane monochromatic waves. Consider a complex $E(z)$, namely $E = \sqrt{\frac{Q}{k_0}}A\mathrm{e}^{\mathrm{i}q}$, where the invariant Q, the dimensionless amplitude $A(z)$ and phase $q(z)$ are real quantities. Inserting this ansatz in (7) leads to the amplitude equation for $A(z)$ [2, 3]

$$\frac{1}{k_0^2}A^3A'' = 1 - n^2A^4, \tag{8}$$

where the prime indicates the derivative with respect to z. The invariant Q establishes a relationship between amplitude and phase, which written for the dimensionless amplitude is

$$q' = \frac{k_0}{A^2}. \tag{9}$$

Equation (8) is an Ermakov–Milne–Pinney type equation [14–16].

If the parameter $\frac{1}{k_0^2}$ is small enough that the terms in (8) satisfy $\frac{1}{k_0^2}|A^3A''| \ll n^2|A^4|$, or equivalently

$$\frac{1}{k_0^2} \ll n^2\left|\frac{A}{A''}\right|, \tag{10}$$

an approximate solution of (8) can be constructed as a power series [6]:

$$A_{\mathrm{SVRI}} = \sum_{m=0}^{\infty} A_m \left(\frac{1}{k_0}\right)^m, \tag{11}$$

where every term of the sum is a function of z, $A_m = A_m(z)$. Substitution of (11) in the nonlinear differential equation (8) yields

$$\frac{1}{k_0^2}\left(\sum_a \frac{A_a}{k_0^a}\right)\left(\sum_b \frac{A_b}{k_0^b}\right)\left(\sum_c \frac{A_c}{k_0^c}\right)\left(\sum_d \frac{A_d''}{k_0^d}\right)$$
$$= 1 - n^2\left(\sum_\alpha \frac{A_\alpha}{k_0^\alpha}\right)\left(\sum_\beta \frac{A_\beta}{k_0^\beta}\right)\left(\sum_\gamma \frac{A_\gamma}{k_0^\gamma}\right)\left(\sum_\delta \frac{A_\delta}{k_0^\delta}\right), \tag{12}$$

where all the summation indices run from 0 to ∞. Equating terms with the same power of k_0 yields, for $k_0^0 = 1$, the value of A_0,

$$0 = 1 - n^2 A_0^4 \quad \Rightarrow \quad A_0 = n^{-\frac{1}{2}}.$$

Then, for k_0^{-1}, the first order amplitude term A_1 is

$$0 = k_0^{-1}\frac{4!}{1!3!}n^2 A_0^3 A_1 \quad \Rightarrow \quad A_1 = 0.$$

Every term with a k_0^{-3} factor includes an A_1, so the value of A_3 is zero. In fact, any other A_m with an odd m is also null. For k_0^{-2}, the second order amplitude term A_2 is

$$A_2 = -\frac{3}{16}n^{-\frac{9}{2}}\left(\frac{\mathrm{d}n}{\mathrm{d}z}\right)^2 + \frac{1}{8}n^{-\frac{7}{2}}\left(\frac{\mathrm{d}^2 n}{\mathrm{d}z^2}\right).$$

Following the same procedure, one can still easily write A_4,

$$A_4 = \frac{621}{512}n^{-\frac{17}{2}}\left(\frac{\mathrm{d}n}{\mathrm{d}z}\right)^4 - \frac{207}{128}n^{-\frac{15}{2}}\left(\frac{\mathrm{d}n}{\mathrm{d}z}\right)^2\left(\frac{\mathrm{d}^2 n}{\mathrm{d}z^2}\right)$$
$$+ \frac{29}{128}n^{-\frac{13}{2}}\left(\frac{\mathrm{d}^2 n}{\mathrm{d}z^2}\right)^2 + \frac{5}{16}n^{-\frac{13}{2}}\left(\frac{\mathrm{d}n}{\mathrm{d}z}\right)\left(\frac{\mathrm{d}^3 n}{\mathrm{d}z^3}\right)$$
$$- \frac{1}{32}n^{-\frac{11}{2}}\left(\frac{\mathrm{d}^4 n}{\mathrm{d}z^4}\right).$$

As even m's value grow, to write explicitly the terms for A_m becomes a strenuous task. Each A_m involves terms including combinations of $n(z)$ derivatives up to the mth order. However, a general recurrence relation for $m > 1$ can be written [6]; in the present case, it is

$$A_m = -\frac{1}{4A_0^3}\left(\sum_{\alpha,\beta,\gamma,\zeta}^{m-2} A_\alpha A_\beta A_\gamma A_\zeta \delta \times [m - (\alpha+\beta+\gamma+\zeta)]\right)$$
$$- \frac{1}{4A_0^3 n^2}\left(\sum_{a,b,c,d}^{m-2} A_a'' A_b A_c A_d \delta[(m-2) - (a+b+c+d)]\right) \tag{13}$$

where δ is a Kronecker delta, which 'turns on' all the index combinations that satisfy $\alpha+\beta+\gamma+\zeta = m$ and $a+b+c+d = m-2$.

3. The highest order derivative term

Further on, when we write the reflection coefficient to leading order, it will be useful to notice that, for every A_m with an even m, at least the single term including the highest order refractive index derivative can be written explicitly in a simple way. From (13) we highlight the term involving the highest order derivative of n, namely with $a = m-2$, $b = c = d = 0$,

$$A_m = -\tfrac{1}{4}n^{-2}A_{m-2}'' + \mathcal{O}(< m). \tag{14}$$

where $\mathcal{O}(< m)$ stands for all the other terms, involving derivatives of the refractive index of lower order than m. Similarly for A_{m-2},

$$A_{m-2} = -\tfrac{1}{4}n^{-2}A_{m-4}'' + \mathcal{O}(< m-2). \tag{15}$$

Inserting (15) in (14),

$$A_m = -\tfrac{1}{4}n^{-2}(-\tfrac{1}{4}n^{-2}A_{m-4}'' + \mathcal{O}(< m-2))'' + \mathcal{O}(< m)$$
$$= -\tfrac{1}{4}n^{-2}(-\tfrac{1}{4}n^{-2}A_{m-4}'''') + \mathcal{O}(< m).$$

Repeating the process $m/2$ times,

$$A_m = \left(-\frac{1}{4}n^{-2}\right)^{\frac{m}{2}}\frac{\mathrm{d}^m A_0}{\mathrm{d}z^m} + \mathcal{O}(< m),$$

for an even m. Since $A_0 = n^{-1/2}$, the factor $\frac{\mathrm{d}^m A_0}{\mathrm{d}z^m}$ has only one term involving the highest derivative of the refractive index. For $m > 0$, $\frac{\mathrm{d}^m A_0}{\mathrm{d}z^m} = -\frac{1}{2}n^{-\frac{3}{2}}\frac{\mathrm{d}^m n}{\mathrm{d}z^m} + \mathcal{O}(< m)$, so

$$A_m = \left(\frac{(-1)^{\frac{m}{2}+1}}{n^{m+\frac{3}{2}}2^{m+1}}\right)\frac{\mathrm{d}^m n}{\mathrm{d}z^m} + \mathcal{O}(< m). \tag{16}$$

The series in (11) converges if, for every m, the parameter k_0^{-2m} is small compared to all the refractive index derivatives up to the mth order, small enough to ensure convergence by the d'Alembert ratio test [17]. This means that $n(z)$ must be analytic in the desired range and vary evenly, at the wavelength scale.

If A_{SVRI} can be written as a series expansion in k_0^{-2}, so its square A_{SVRI}^2,

$$A_{\mathrm{SVRI}}^2 = \sum_{j=0}^{\infty} A_{2j}k_0^{-2j}\sum_{l=0}^{\infty} A_{2l}k_0^{-2l}. \tag{17}$$

Writing the first few terms explicitly,

$$A_{\mathrm{SVRI}}^2 = A_0^2 + 2A_0A_2k_0^{-2} + (2A_0A_4 + A_2A_2)k_0^{-4} + \cdots$$
$$+ \left(\sum_{j=0}^{m} A_{2j}A_{m-2j}\right)k_0^{-m} + \cdots, \tag{18}$$

where m is an even integer greater than zero. Each order of the series expansion involves a group of terms; we highlight again the term involving the highest order derivative of n,

$$[A_{\mathrm{SVRI}}^2]_m = \left(\frac{(-1)^{\frac{m}{2}+1}}{n^{m+2}2^m}\right)\frac{\mathrm{d}^m n}{\mathrm{d}z^m} + \mathcal{O}(< m). \tag{19}$$

Similarly, for its derivative,

$$\frac{\mathrm{d}[A^2_{\mathrm{SVRI}}]_m}{\mathrm{d}z} = \left(\frac{(-1)^{\frac{m}{2}+1}}{n^{m+2}2^m}\right)\frac{\mathrm{d}^{m+1}n}{\mathrm{d}z^{m+1}} + \mathcal{O}(< m+1). \quad (20)$$

4. Counter-propagating solution of the field equation based on the SVRI approximation

We should recall that this SVRI solution A_{SVRI} is only a particular and approximate solution; it does not oscillate when n is constant. For example, if we were to use it with the all analytic Epstein $n(z)$ profile (1), reflectivity would be zero for every s value. To achieve an oscillating $A(z)$ we can recall the linear superposition principle for solutions of the field equation (7)

$$E_{\mathrm{SVRI}}(z) = A_{\mathrm{SVRI}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{SVRI}}} + \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{SVRI}}}), \quad (21)$$

where $\tilde{A}_i$ and $\tilde{A}_r$ are complex constants. Notice that this reveals the existence of a nonlinear superposition rule for the amplitude equation (8) solutions [18], since the modulus $A = |E_{\mathrm{SVRI}}(z)|$ of (21) solves the following equation:

$$\frac{\mathrm{d}^2A}{\mathrm{d}z^2} - \frac{k_0^2(A_i^2 - A_r^2)^2}{A^3} = -k_0^2 n^2 A, \quad (22)$$

where $A_i^2 = \tilde{A}_i{}^*\tilde{A}_i$ and $A_r^2 = \tilde{A}_r{}^*\tilde{A}_r$.

Equation (9) allows us to find an SVRI approximated expression for the phase q,

$$q_{\mathrm{SVRI}} = \int \frac{k_0}{A^2_{\mathrm{SVRI}}}\mathrm{d}z. \quad (23)$$

4.1. Joining the solutions

To attain a non-vanishing reflectivity a single piecewise junction will be introduced; the reflection coefficient thus obtained will be a consequence of the junction only. We consider again a monotonic continuous profile $n(z)$ that evolves from n_i to n_t; this profile is constructed by piecewise joining two functions at z_0. On both sides of the junction, $n(z)$ is analytic and slowly varying so the SVRI approximation is valid. Light is incident from the left, so this region may have counter-propagating waves due to reflection. To the right of the junction plane, only a transmitted wave propagates to the right, as shown in figure 1.

The field equation solution for the counter-propagating region to the left of the discontinuous derivative at $z = z_0 = 0$ is

$$E(z)_{\mathrm{left}} = A_{\mathrm{left}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}} + \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}}), \quad (24)$$

where A_{left} is the SVRI approximate solution for the $n(z)$ profile to the left of the junction. Similarly, to the right of the junction at $z = 0$,

$$E(z)_{\mathrm{right}} = A_{\mathrm{right}}\tilde{A}_t \mathrm{e}^{\mathrm{i}q_{\mathrm{right}}}, \quad (25)$$

where A_{right} is the SVRI approximate solution for the $n(z)$ profile to the right of the junction and $\tilde{A}_t$ is another complex

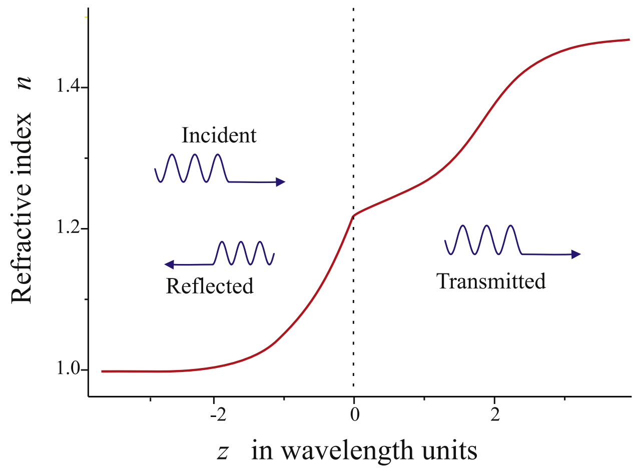

Figure 1. A monotonic continuous profile $n(z)$ that evolves from n_i to n_t. Two slowly varying functions are piecewise joined at $z = z_0 = 0$. Light is incident from the left, so the region on the left of the junction may have counter-propagating waves due to reflection. The region on the right will only have a transmitted wave propagating to the right.

constant. Boundary conditions require continuous electric E and magnetic H fields across the junction, at z_0,

$$A_{\mathrm{left}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}} + \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}}) = A_{\mathrm{right}}\tilde{A}_t \mathrm{e}^{\mathrm{i}q_{\mathrm{right}}},$$
$$A'_{\mathrm{left}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}} + \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}}) + \mathrm{i}A_{\mathrm{left}}q'_{\mathrm{left}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}} - \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}})$$
$$= (A'_{\mathrm{right}} + \mathrm{i}q'_{\mathrm{right}}A_{\mathrm{right}})\tilde{A}_t \mathrm{e}^{\mathrm{i}q_{\mathrm{right}}}. \quad (26)$$

This last equation can be rewritten after a few algebraic operations and using (23),

$$A_{\mathrm{left}}(\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}} - \tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}}) = \left[\frac{\mathrm{i}}{k_0}\frac{A_{\mathrm{left}}}{A_{\mathrm{right}}}(A'_{\mathrm{left}}A_{\mathrm{right}} - A_{\mathrm{left}}A'_{\mathrm{right}}) + \frac{A^2_{\mathrm{left}}}{A^2_{\mathrm{right}}}\right]A_{\mathrm{right}}\tilde{A}_t \mathrm{e}^{\mathrm{i}q_{\mathrm{right}}}. \quad (27)$$

By adding (26) and (27) the transmission coefficient t can be found:

$$t = \frac{A_{\mathrm{right}}\tilde{A}_t \mathrm{e}^{\mathrm{i}q_{\mathrm{right}}}}{A_{\mathrm{left}}\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}}} = \frac{2A^2_{\mathrm{right}}}{A^2_{\mathrm{right}} + A^2_{\mathrm{left}} + \frac{\mathrm{i}}{2k_0}\left(A^2_{\mathrm{right}}\frac{\mathrm{d}A^2_{\mathrm{left}}}{\mathrm{d}z} - A^2_{\mathrm{left}}\frac{\mathrm{d}A^2_{\mathrm{right}}}{\mathrm{d}z}\right)}. \quad (28)$$

Subtracting (26) and (27), along with (28), leads to the reflection coefficient

$$r = \frac{A_{\mathrm{left}}\tilde{A}_r \mathrm{e}^{-\mathrm{i}q_{\mathrm{left}}}}{A_{\mathrm{left}}\tilde{A}_i \mathrm{e}^{\mathrm{i}q_{\mathrm{left}}}} = \frac{A^2_{\mathrm{right}} - A^2_{\mathrm{left}} - \frac{\mathrm{i}}{2k_0}\left(A^2_{\mathrm{right}}\frac{\mathrm{d}A^2_{\mathrm{left}}}{\mathrm{d}z} - A^2_{\mathrm{left}}\frac{\mathrm{d}A^2_{\mathrm{right}}}{\mathrm{d}z}\right)}{A^2_{\mathrm{right}} + A^2_{\mathrm{left}} + \frac{\mathrm{i}}{2k_0}\left(A^2_{\mathrm{right}}\frac{\mathrm{d}A^2_{\mathrm{left}}}{\mathrm{d}z} - A^2_{\mathrm{left}}\frac{\mathrm{d}A^2_{\mathrm{right}}}{\mathrm{d}z}\right)}. \quad (29)$$

Let us recall that, in equations (26)–(29), the quantities A_{right}, A_{left} and their derivatives are evaluated infinitesimally close to z_0. The reflection coefficient in (29) is due only to the junction at $z = 0$; reflectivity from the rest of the refractive index profile is negligible as long as the SVRI approximation is valid.

5. Evaluation of the reflection coefficient

In this section, we evaluate the reflection coefficient to leading order, for different profile types. Notice that r is a quotient of two Taylor series in powers of $\frac{1}{k_0}$. This quotient may also be expressed as a power series of $\frac{1}{k_0}$,

$$\begin{aligned} r &= \frac{a_0 + a_1 k_0^{-1} + a_2 k_0^{-2} + \cdots}{b_0 + b_1 k_0^{-1} + b_2 k_0^{-2} + \cdots} \\ &= r_0 + r_1 k_0^{-1} + r_2 k_0^{-2} + \cdots, \end{aligned} \tag{30}$$

where the as and bs are the coefficients of the numerator and denominator respectively. Performing a polynomial long division, a recurrence relation can be written for the rs,

$$\begin{aligned} r_0 &= \frac{a_0}{b_0}, \qquad r_1 = \frac{a_1 - r_0 b_1}{b_0}, \\ r_2 &= \frac{a_2 - r_0 b_2 - r_1 b_1}{b_0}, \\ r_3 &= \frac{a_3 - r_0 b_3 - r_1 b_2 - r_2 b_1}{b_0} \end{aligned} \tag{31}$$

and for the jth term,

$$r_j = \frac{a_j}{b_0} - \sum_{l=0}^{j-1} \frac{r_l b_{j-l}}{b_0}. \tag{32}$$

Inspection of (29) allows us to see that the first two terms of both numerator and denominator, yield the even order terms for as and bs since A^2_{SVRI} and its derivative only include terms of even order in $\frac{1}{k_0}$. The as and bs are, for an even order,

$$\begin{aligned} a_{2j} &= [A^2_{\mathrm{right}}]_{2j} - [A^2_{\mathrm{left}}]_{2j}, \\ b_{2j} &= [A^2_{\mathrm{right}}]_{2j} + [A^2_{\mathrm{left}}]_{2j}, \end{aligned} \tag{33}$$

where $[A^2_{\mathrm{right}}]_{2j}$ and $[A^2_{\mathrm{left}}]_{2j}$ stand for the terms of order $2j$ of the series (18). The factor $\frac{\mathrm{i}}{2k_0}$ in the last two terms of both numerator and denominator in (29) produces the odd order terms for as and bs. These last two terms are products of an A^2_{SVRI} and its derivative, allowing several combinations for a certain order $2j+1$. Then, for an odd order $2j+1$,

$$\begin{aligned} a_{2j+1} = -b_{2j+1} = -\frac{\mathrm{i}}{2} \sum_{l=0}^{j} \Bigg(& [A^2_{\mathrm{right}}]_{2l} \left[\frac{\mathrm{d}A^2_{\mathrm{left}}}{\mathrm{d}z}\right]_{2(j-l)} \\ & - [A^2_{\mathrm{left}}]_{2l} \left[\frac{\mathrm{d}A^2_{\mathrm{right}}}{\mathrm{d}z}\right]_{2(j-l)} \Bigg). \end{aligned} \tag{34}$$

Considering that the refractive index profile is continuous, that is $n_{\mathrm{left}} = n_{\mathrm{right}}$, a first few explicit terms for as and bs can be written briefly,

$$\begin{aligned} a_0 &= 0, \qquad a_1 = \frac{\mathrm{i}}{2n^3}(n'_{\mathrm{left}} - n'_{\mathrm{right}}), \\ a_2 &= \tfrac{3}{8} n^{-5}(n'^2_{\mathrm{left}} - n'^2_{\mathrm{right}}) + \tfrac{1}{4} n^{-4}(n''_{\mathrm{right}} - n''_{\mathrm{left}}), \end{aligned} \tag{35}$$

$$b_0 = 2n^{-1}, \qquad b_1 = -\frac{\mathrm{i}}{2n^3}(n'_{\mathrm{left}} - n'_{\mathrm{right}}),$$

$$b_2 = -\tfrac{3}{8} n^{-5}(n'^2_{\mathrm{left}} + n'^2_{\mathrm{right}}) + \tfrac{1}{4} n^{-4}(n''_{\mathrm{right}} + n''_{\mathrm{left}}). \tag{36}$$

Complete sets of higher order terms may not be as briefly written, but fortunately, further on we will focus our attention only on the terms involving the highest derivative order of the refractive index. Following (19), as for an even order are

$$a_{2j} = \left(\frac{\mathrm{i}^{2j+2}}{n^{(2j+2)} 2^{2j}}\right) \left(\frac{\mathrm{d}^{2j} n_{\mathrm{right}}}{\mathrm{d}z^{2j}} - \frac{\mathrm{d}^{2j} n_{\mathrm{left}}}{\mathrm{d}z^{2j}}\right) + \mathcal{O}(< 2j), \tag{37}$$

where we inserted $\mathrm{i}^2 = -1$. For an odd order, we choose only $l = 0$ of the sum in (34), since that set of terms contains the highest derivative order of $n(z)$,

$$\begin{aligned} a_{2j+1} = -\frac{\mathrm{i}}{2}[A^2]_0 \left(\frac{\mathrm{i}^{2j+2}}{n^{2j+2} 2^{2j}}\right) \left(\frac{\mathrm{d}^{2j+1} n_{\mathrm{left}}}{\mathrm{d}z^{2j+1}} - \frac{\mathrm{d}^{2j+1} n_{\mathrm{right}}}{\mathrm{d}z^{2j+1}}\right) \\ + \mathcal{O}(< 2j+1), \end{aligned} \tag{38}$$

where we have used (20). Simplifying this last equation yields

$$\begin{aligned} a_{2j+1} = \left(\frac{\mathrm{i}^{2j+3}}{n^{2j+3} 2^{2j+1}}\right) \left(\frac{\mathrm{d}^{2j+1} n_{\mathrm{right}}}{\mathrm{d}z^{2j+1}} - \frac{\mathrm{d}^{2j+1} n_{\mathrm{left}}}{\mathrm{d}z^{2j+1}}\right) \\ + \mathcal{O}(< 2j+1); \end{aligned} \tag{39}$$

substituting $2j+1$ for $2j$ allows us to see that (37) and (39) are equivalent.

Refractive index profiles can be categorized depending on the lowest order discontinuous derivative. A C^j type profile means that $n(z)$ is continuous as well as its derivatives except for the $j+1$ order derivative $\frac{\mathrm{d}^{j+1} n}{\mathrm{d}z^{j+1}}$ and possibly higher orders [19]. This profile classification allows us to write the reflection coefficient in a fairly simple way.

5.1. Type C^0 profile

The refractive index profile is continuous but not its first and possibly higher order derivatives at the junction. Since a_0 vanishes, thus $r_0 = 0$, the reflection coefficient lowest non-vanishing term is of first order,

$$r \approx r_1 k_0^{-1} = \frac{a_1}{b_0} k_0^{-1} = \mathrm{i}\frac{n'_{\mathrm{left}} - n'_{\mathrm{right}}}{4 k_0 n^2}. \tag{40}$$

The last equality follows from (31) and (35).

5.2. Type C^1 profile

The refractive index profile and its first derivative are continuous but not the second and possibly higher order derivatives at the junction. This means that a_0 and a_1 vanish as well as r_0 and r_1. This time the reflection coefficient leading order term is of second order,

$$r \approx r_2 k_0^{-2} = \frac{a_2}{b_0} k_0^{-2}, \tag{41}$$

following from (31). The quantity a_2 is a sum of two couple of terms, one couple involving the first derivative of the refractive index and the other the second derivative. The terms involving first derivatives of the refractive index in (35) cancel. Only the terms involving the highest order derivative of the refractive index in the numerator will not cancel, so

$$r \approx \frac{n''_{\text{right}} - n''_{\text{left}}}{8k_0^2 n^3}. \tag{42}$$

5.3. Type C^2 profile

The refractive index profile, its first derivative and the second are continuous, but not the third and possibly higher order derivatives at the junction. This time a_0, a_1 and a_2 vanish along with r_0, r_1 and r_2. The reflection coefficient leading order term is of third order,

$$r \approx r_3 k_0^{-3} = \frac{a_3}{b_0} k_0^{-3}. \tag{43}$$

Since $n'_{\text{right}} = n'_{\text{left}}$ and $n''_{\text{right}} = n''_{\text{left}}$ at the junction, the terms of a_3 involving first and second derivatives of the refractive index in (34) vanish. This leaves only the terms involving the higher order derivatives, the ones highlighted in (38)

$$r \approx \mathrm{i}\frac{n'''_{\text{right}} - n'''_{\text{left}}}{16k_0^3 n^4}. \tag{44}$$

5.4. Type C^{2j-1} and C^{2j} profiles

For a C^{2j-1} profile, the refractive index along with all its derivatives up to order $2j-1$ are continuous; $2j$ and possibly higher order derivatives are not at the junction. Then $a_0, a_1, \ldots, a_{2j-1}$ vanish along with $r_0, r_1, \ldots, r_{2j-1}$. The leading order term of the reflection coefficient is of $2j$ order; then

$$r \approx r_{2j} k_0^{-2j} = \frac{a_{2j}}{b_0} k_0^{-2j}. \tag{45}$$

Since $\frac{\mathrm{d}^m n_{\text{right}}}{\mathrm{d}z^m} = \frac{\mathrm{d}^m n_{\text{left}}}{\mathrm{d}z^m}$ for $m = 1, 2, 3, \ldots, 2j-1$ at the junction, the terms involving refractive index derivatives of $2j-1$ order and lower in the first of equations (33) cancel. This leaves only the terms involving $2j$ order derivatives; equation (37) allows us to write these terms

$$r \approx \left(\frac{\mathrm{i}^{2j+2}}{2^{2j+1} k_0^{2j} n^{2j+1}}\right)\left(\frac{\mathrm{d}^{2j} n_{\text{right}}}{\mathrm{d}z^{2j}} - \frac{\mathrm{d}^{2j} n_{\text{left}}}{\mathrm{d}z^{2j}}\right). \tag{46}$$

Similarly for a C^{2j} profile,

$$r \approx r_{2j+1} k_0^{-2j+1} = \frac{a_{2j+1}}{b_0} k_0^{-2j-1}. \tag{47}$$

Since $\frac{\mathrm{d}^g n_{\text{right}}}{\mathrm{d}z^g} = \frac{\mathrm{d}^g n_{\text{left}}}{\mathrm{d}z^g}$ for $g = 1, 2, 3, \ldots, 2j$ at the junction, the terms involving $2j$ and lower order derivatives of the refractive index in (34) cancel. This leaves only the terms involving $2j+1$ order derivatives; equation (38) allows us to write these terms as

$$r \approx \left(\frac{\mathrm{i}^{2j+3}}{n^{2j+2} k_0^{2j+1} 2^{2j+2}}\right)\left[\frac{\mathrm{d}^{2j+1} n_{\text{right}}}{\mathrm{d}z^{2j+1}} - \frac{\mathrm{d}^{2j+1} n_{\text{left}}}{\mathrm{d}z^{2j+1}}\right]; \tag{48}$$

again exchanging $2j+1$ for $2j$ in this last equation, it is seen that equations (46) and (48) are equivalent. So, for either even or odd j in C^j, the reflection coefficient to leading order is written as

$$r \approx \left(\frac{\mathrm{i}^{j+3}}{n^{j+2} k_0^{j+1} 2^{j+2}}\right)\left[\frac{\mathrm{d}^{j+1} n_{\text{right}}}{\mathrm{d}z^{j+1}} - \frac{\mathrm{d}^{j+1} n_{\text{left}}}{\mathrm{d}z^{j+1}}\right]. \tag{49}$$

6. Reflection enhancement

In order to exhibit the reflection enhancement due to discontinuities in the derivative of the refractive index, let us compare smooth functions with their counterparts having discontinuities. To this end, consider smooth hyperbolic tangent functions of the form given by (1), and on the other hand continuous piecewise functions, constructed by joining two originally smooth functions with a discontinuous derivative at their junction.

In figure 2, four different examples of refractive index profile types are plotted [1]: C^0 is built by joining a hyperbolic tangent with a linear function, C^1 is produced with a squared hyperbolic secant joined to a linear function, C^2 is produced with a cubic exponential joined to a linear function and C^3 is built by joining quartic exponential with a linear function. All of them are shown along with a hyperbolic tangent function (Epstein profile) with $s = 1.75$, $s = 2.07$, $s = 2.23$ and $s = 2.21$ respectively. Each couple is matched so that their maximum gradient $n'_{\max}$ is the same; derivative discontinuities are always placed at $z = 0$. Reflectivities for the piecewise, derivative discontinuous functions are calculated with the final result abridged in equation (49). For the smooth functions, the reflectivity is evaluated using the expression involving hyperbolic sines in (2); these results are compared in table 1. Although the C^0 profile shows a more gradual rise than the smooth match, its reflectivity is 2.75×10^5 times greater due to the derivative discontinuity at the junction. As the order of the leading discontinuous derivative becomes higher, the couples look more alike and the difference between their reflectivities becomes smaller, yet it is still significant. A derivative discontinuity within a continuous refractive index profile clearly enhances reflection significantly. These are just a few particular examples, but they show the general behavior.

7. Comparison between numeric and analytic results

The complex reflection coefficients r for the examples shown in figure 2 are listed in table 2. The numerical results were obtained from the amplitude equation (8) numerical solutions [1]. These solutions were attained by a finite

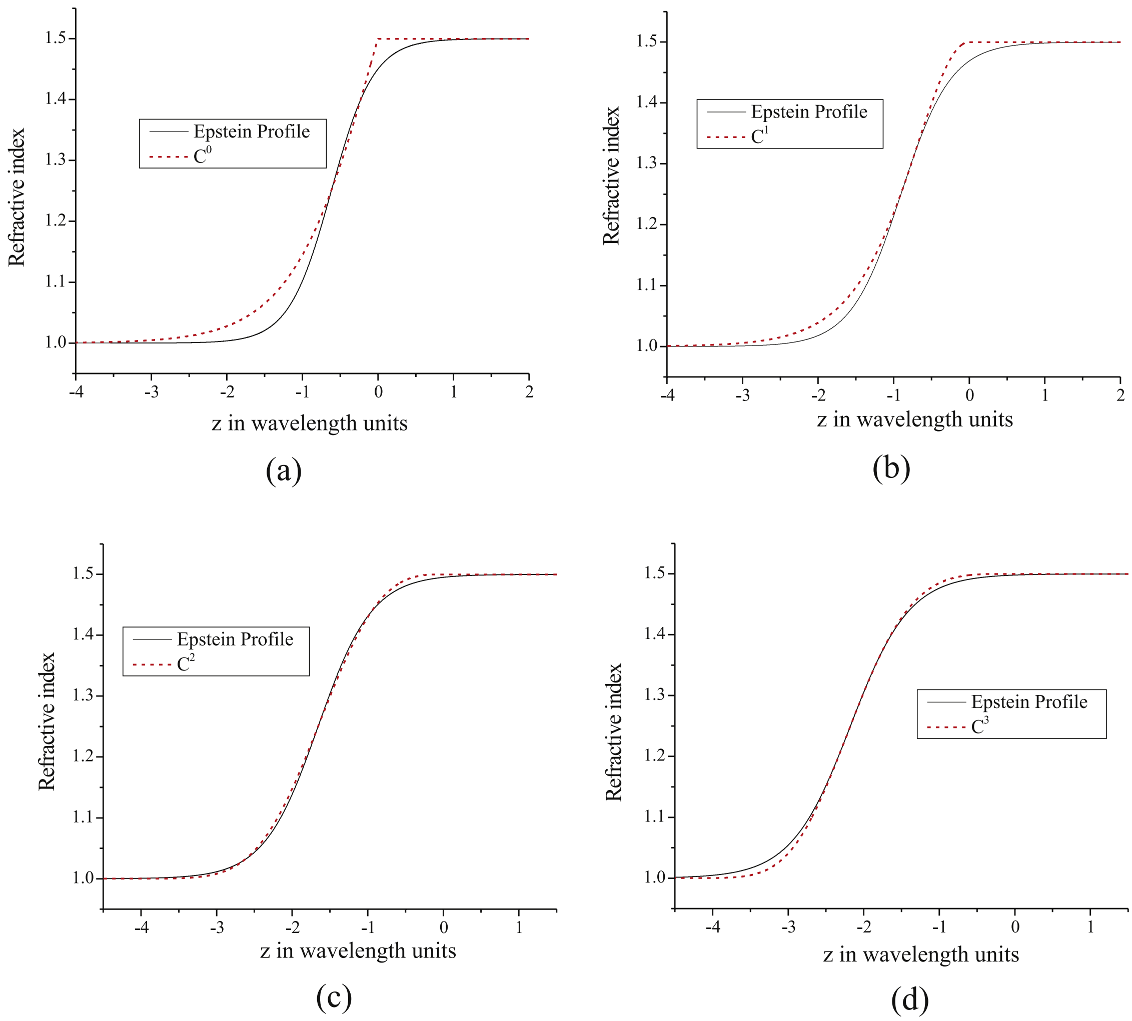

Figure 2. (a) Discontinuous first derivative, a C^0 refractive index profile. (b) Discontinuous second derivative, a C^1 refractive index profile. (c) A type C^2 refractive index profile. (d) A type C^3 refractive index profile. A smooth hyperbolic tangent function (Epstein profile in solid black) is superimposed on each curve.

Table 1. Reflectivities for piecewise [1] and discontinuity-free profiles. The profile type for the piecewise case and parameter s for the hyperbolic tangent function profile are indicated.

	Reflectivity (%)			
	C^0 and $s = 1.75$	C^1 and $s = 2.07$	C^2 and $s = 2.23$	$C^3$and $s = 2.44$
Piecewise	6.27×10^{-3}	8.15×10^{-5}	5.15×10^{-8}	2.09×10^{-10}
Epstein profile	2.28×10^{-8}	5.03×10^{-10}	6.74×10^{-11}	4.82×10^{-12}

difference method; no explicit approximation was used regarding how gradually the refractive index changes with z. Deviations for the numerical results are very small or not relevant so they are omitted. The analytic results were estimated with (49). There is a great similarity between the numeric and analytic outcomes. For the modulus, the difference is within 1% for the $C^0 - C^2$ profiles. When the reflectivity becomes very small, the modulus relative difference becomes somewhat larger. Regarding the phase, deviations of the numerical results from the analytic value are 1% or less for the $C^0 - C^2$ profiles. For the very low C^3 reflectivity, the phase difference is 3%.

Regarding the analytical results, departure from the reflection coefficient actual true value is due to two factors: (i) we only kept the leading order term of the SVRI expansion and (ii) reflection from the smooth part of the profile was neglected. Inaccuracy of the numerical results is due to the discretization steps: the actual continuous $n(z)$ profile is replaced by discrete points in order to apply the finite difference method. The derivative discontinuity at the junction can be viewed as a larger discontinuity compared to the ones introduced by discretization.

As j increases with the profile type C^j, the modulus of r in (49) decreases and the reflectivity of the smooth part of the profile becomes comparable. On the other hand, if j

Table 2. Modulus and phase of the complex reflection coefficient r, evaluated for the functions shown in figure 2. The present analytical results are remarkably similar to previous numerical calculations also reproduced in this table.

		r complex reflection coefficient			
		$n(z)$ profile type			
		C^0	C^1	C^2	C^3
Analytic	Modulus	7.88×10^{-3}	8.93×10^{-4}	2.29×10^{-5}	9.85×10^{-7}
	Phase	$\frac{\pi}{2}$	0	$\frac{\pi}{2}$	$-\pi$
Numeric [1]	Modulus	7.92×10^{-3}	9.03×10^{-4}	2.27×10^{-5}	1.44×10^{-6}
	Phase	$\frac{\pi}{2} + \frac{\pi}{224}$	$\frac{\pi}{1571}$	$\frac{\pi}{2} - \frac{\pi}{785}$	$-\pi - \frac{\pi}{31}$

is large enough, the junction derivative discontinuity starts to be comparable to the discretization discontinuities. For both the numerical and the analytical methods, accuracy to yield the reflection coefficient of the whole profile is expected to diminish as j increases. The greater relative difference between results obtained with these methods for C^3 may be a consequence. The approximation to leading order of (49) affects all profile types the same. In relation to the phase, if we consider higher order terms, small deviations from the integer and half integer values of π are expected from the analytical results since they alternate from real to imaginary.

8. Consistency with earlier exact solutions and applications

There are other known reflection coefficients for particular cases of continuous $n(z)$ with a derivative discontinuity; some examples are recalled in section 1.1. The profile introduced by Wallot and Försterling [11, 20] and its reflection coefficient for slowly varying refractive index (later reviewed by Brekhovskikh [7]) are shown in equations (5) and (6). This profile is the result of joining, at $z = 0$, a homogeneous medium with one that presents an increasing linear behavior ($a < 0$) for the relative permittivity; it corresponds to a C^0 profile. Based on (5) one can write the value of the constant parameter a as $a = 2n'_{\text{right}}(z = 0)$, substituting in (6)

$$r = -\frac{\mathrm{i}n'_{\text{right}}}{4k_0\cos^3\theta_0}.$$

For normal incidence, $\cos^3\theta_0 = 1$, $n(z = 0) = 1$ and $n'_{\text{left}} = 0$ for the homogeneous medium to the left, this last equation is consistent with (40).

The Rayleigh profile in equation (3) is a C^0 too. By letting $\frac{1}{ak_0} \ll 1$, that is, by considering a slowly varying refractive index, equation (4) reduces to

$$r \approx \frac{\mathrm{i}}{4k_0 a}. \tag{50}$$

The constant a can be related to the refractive index gradient to the right of the junction $n'_{\text{right}}/n^2_{\text{right}} = -\frac{1}{a}$; then equation (50) becomes

$$r \approx -\mathrm{i}\frac{n'_{\text{right}}}{4k_0 n^2}.$$

This particular case is again consistent with (40) since $n'_{\text{left}} = 0$. The last two examples include a discontinuity in the first derivative of the refractive index and the junction involved binds a particular inhomogeneous medium with a homogeneous one.

As the order of the lowest order discontinuous derivative becomes greater, reflectivity drops. This fact explains, for example, why the so called quintic anti-reflective films (a C^2 type profile) work well [21]. One may think that a C^3 layer could work better but, in order to keep a slowly varying refractive index, that layer would have to be thicker, a characteristic that is not always desirable.

Combinations of various reflection planes of this sort may be used to build dielectric mirrors, anti-reflective coatings or filters [22]. For example, the junction of a triangular shape $n(z)$ profile, with a gradient of $|\frac{\mathrm{d}n}{\mathrm{d}z}| = \frac{3.5}{\lambda}$ on both sides, may provide a reflectivity of $R = 1.53\%$, while the two side linear functions still ensure SVRI series convergence. However, as we have stressed since previous communications, experimental confirmation of these predictions would be highly welcomed.

9. Conclusions

The complex reflection coefficient for discontinuities in the mth order derivative of the refractive index profile has been obtained in closed analytical form to leading order in the SVRI approximation. The expression is simple and depends on the lowest order discontinuous derivative on both sides of the junction. We have shown that the reflectivity is greatly enhanced at the derivative discontinuity plane even if the refractive index is continuous. The reflectivity due to this discontinuity can be several orders of magnitude larger than that of the smooth part of the $n(z)$ profile. The reflectivity diminishes as the lowest order of the discontinuous derivative increases.

Regarding the phase, the proposition that 'For a C^j refractive index profile type, phase change upon reflection at the discontinuity plane is $(1 - j)\frac{\pi}{2}$ for an increasing lowest order discontinuous derivative and $(-1 - j)\frac{\pi}{2}$ for the decreasing case' has been proved. In addition to the usual 0 or π phase shift obtained from the Fresnel equations for discontinuous dielectric media, $\pm\pi/2$ phase changes upon reflection can also be obtained if $\left(\mathrm{d}^{2m}n/\mathrm{d}z^{2m}\right)$ is discontinuous. The sign of the phase shift depends on whether the derivative of n increases or decreases, as may be seen from (49). This equation can be thought of as a generalization of the Fresnel relations, for normal incidence, when the derivatives of $n(z)$ rather than the refractive index itself are discontinuous. The present analytical results have been compared with previous numerical results. Predictions with both methods are remarkably similar for both the modulus and phase of the complex reflection coefficient. Other known theoretical results are consistent with our predictions too.

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