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Extrema of the magnitude and the phase of a complex function of a real variable: application to attenuated internal reflection

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Given a complex function $F(\omega) = |F(\omega)|\exp[j\Delta(\omega)]$ of a real argument ω, the extrema of its magnitude $|F(\omega)|$ and its phase $\Delta(\omega)$, as functions of ω, are determined simultaneously by finding the roots of one common equation, $\mathrm{Im}[G(\omega)] = 0$, where $G = (F'/F)^2$ and $F' = \partial F/\partial\omega$. The extrema of $|F|$ and Δ are associated with Re $G < 0$ and Re $G > 0$, respectively. This easy-to-prove theorem has a wide range of applications in physical optics. We consider attenuated internal reflection (AIR) as an example. In AIR the complex reflection coefficient for the p polarization, $r_p(\phi)$, and the ratio of complex reflection coefficients for the p and s polarizations, $\rho(\phi) = r_p(\phi)/r_s(\phi)$, are considered as functions of the angle of incidence ϕ. It is found that the same (cubic) equation that determines the pseudo-Brewster angle of minimum $|r_p|$ also determines a new angle at which the reflection phase shift $\delta_p = \arg r_p$ exhibits a minimum of its own. Likewise, the same (quartic) equation that determines the second Brewster angle of minimum $|\rho|$ also determines angles of incidence at which the differential reflection phase shift $\Delta = \arg \rho$ experiences a minimum and a maximum. Angular positions and magnitudes of all extrema are calculated exactly for a specific case that represents light reflection by the vacuum–Al or glass–aqueous-dye-solution interface. As another example, the normal-incidence reflection of light by a birefringent film on an absorbing substrate is examined. The ratio of complex principal reflection coefficients is considered as a function of the film thickness normalized to the wavelength of light. The absolute value and the phase of this function exhibit multiple extrema, the first 13 of which are determined for a specific birefringent film on a Si substrate.

1. INTRODUCTION

Complex functions of real arguments abound in physical optics and electrical engineering. They arise when one considers the steady-state response of a linear system to a time-harmonic (sinusoidal) excitation. The transfer function, defined as the ratio of the complex amplitude of the response to that of the excitation, is a complex function $F(\omega, p_k)$ of the excitation frequency ω and of system parameters p_k ($k = 1, 2, 3, \ldots$). It is natural to write $F = |F|\exp(j\Delta)$, where $|F|$ denotes the amplitude response and Δ denotes the phase response. If $|F|$ and Δ are plotted as functions of ω or p_k, one may encounter maxima and minima that represent the salient features of these functions. In this paper a simple theorem[1] is used to provide an efficient means of locating jointly the extrema of the amplitude and phase responses. As a preliminary application of this theorem, its usefulness is demonstrated in elucidating and analytically determining the extrema of the phase-response functions associated with the attenuated internal reflection (AIR) of a monochromatic plane wave of light at the interface between two media. Finally, another example is given of light reflection at normal incidence by a Si substrate coated by a birefringent film of variable thickness.

2. PROOF OF A SIMPLE THEOREM

Let

$$F(\omega) = |F(\omega)|\exp[j\Delta(\omega)] \tag{1}$$

be a complex function of a real argument ω, expressed in terms of its magnitude (absolute value) $|F(\omega)|$ and its phase (angle) $\Delta(\omega)$. Take the derivative of the natural logarithm of both sides of Eq. (1) to obtain

$$\partial(\ln F)/\partial\omega = F'/F = (|F|'/|F|) + j\Delta', \tag{2}$$

where the prime indicates the first partial derivative with respect to ω, which is suppressed for simplicity. Define the function G as

$$G = (F'/F)^2, \tag{3}$$

and expand the square of the right-hand side of Eq. (2) to get

$$\mathrm{Re}\, G = (|F|'/|F|)^2 - (\Delta')^2, \tag{4}$$

$$\mathrm{Im}\, G = 2(|F|'/|F|)\Delta'. \tag{5}$$

The extrema of $|F|$ and Δ as functions of ω occur when

$$|F|' = 0, \qquad \Delta' = 0, \tag{6}$$

respectively. If we exclude the case when $|F|$ and $|F|'$ vanish simultaneously, Eqs. (5) and (6) give

$$\mathrm{Im}[G(\omega)] = 0, \tag{7}$$

where the argument ω has been reinstated for clarity.

The roots ω_k ($k = 1, 2, \ldots$) of Eq. (7) determine the extrema of the magnitude and phase functions. From Eq. (4) it is noted that

$$\mathrm{Re}\, G < 0 \qquad \text{if } |F|' = 0, \tag{8}$$

$$\mathrm{Re}\, G > 0 \qquad \text{if } \Delta' = 0. \tag{9}$$

Therefore relations (8) and (9) permit the distinction of the extrema of $|F|$ from those of Δ.

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To summarize, given a complex function $F(\omega) = |F(\omega)| \exp[j\Delta(\omega)]$ of a real argument ω, the extrema of its magnitude $|F(\omega)|$ and its phase $\Delta(\omega)$ as functions of ω are determined simultaneously by finding the roots of one common equation, $\mathrm{Im}[G(\omega)] = 0$, where $G = (F'/F)^2$ and $F' = \partial F/\partial\omega$. The extrema of $|F|$ and Δ are associated with Re $G < 0$ and Re $G > 0$, respectively. The significance and usefulness of this simple theorem do not appear to have been recognized previously in physical optics or electrical engineering. It applies, of course, when the function F has several arguments, by considering one variable at a time. A variant of the theorem, when F is expressed in terms of its real and imaginary parts, is developed in Appendix A.

3. APPLICATION TO ATTENUATED INTERNAL REFLECTION

A. Reflection Coefficient for the p Polarization

Consider the reflection of a monochromatic plane wave of light at the planar interface between two homogeneous, linear, nonmagnetic, and isotropic media of dielectric constants ϵ_0 and ϵ_1. The complex amplitude-reflection coefficient for the parallel p (TM) polarization at an angle of incidence ϕ is given by[2]

$$r_p(\phi) = \frac{\epsilon \cos\phi - (\epsilon - \sin^2\phi)^{1/2}}{\epsilon \cos\phi + (\epsilon - \sin^2\phi)^{1/2}}, \tag{10}$$

where

$$\epsilon = \epsilon_1/\epsilon_0 \tag{11}$$

is the complex relative dielectric constant. We assume a transparent medium of incidence (ϵ_0 real) and an absorbing medium of refraction (ϵ_1 complex). If we put

$$\epsilon = \epsilon_r - j\epsilon_i, \tag{12}$$

the condition of AIR implies that

$$0 < \epsilon_r < 1, \qquad \epsilon_i/\epsilon_r \ll 1. \tag{13}$$

If we write

$$r_p = |r_p|\exp(j\delta_p), \tag{14}$$

the extrema of the amplitude reflectance $|r_p|$ and the AIR phase shift δ_p as functions of ϕ are determined by

$$\mathrm{Im}(r_p'/r_p)^2 = 0, \tag{15}$$

according to Eqs. (3) and (7).

It was shown previously[3] that Eq. (15) leads to a cubic equation,

$$\alpha_3 u^3 + \alpha_2 u^2 + \alpha_1 u + \alpha_0 = 0, \tag{16}$$

where

$$u = \sin^2\phi \tag{17}$$

and the coefficients of the cubic are determined by complex ϵ as follows:

$$\alpha_0 = |\epsilon|^4, \qquad \alpha_1 = -2\,|\epsilon|^4,$$
$$\alpha_2 = |\epsilon|^4 - 3|\epsilon|^2, \qquad \alpha_3 = 2\epsilon_r + 2|\epsilon|^2. \tag{18}$$

Other equations that are equivalent to Eq. (16) were derived previously.[4,5]

Whereas Eq. (16) was recognized previously to give the pseudo-Brewster angle of minimum parallel reflectance, it appears that no one has considered the possibility that the same equation could yield other physically meaningful roots. However, Eq. (16) follows from Eq. (15), and, based on the theorem given in Section 2, we conclude that Eq. (16) also determines the angular positions of the extrema of the reflection phase shift δ_p, if they exist. This is indeed the case in AIR, as is demonstrated by the following example.

Let

$$\epsilon = 0.64 - j0.024. \tag{19}$$

One can identify several interfaces between two media that may be characterized with this relative dielectric constant at certain wavelengths. For example, this ϵ represents the vacuum–Al interface[6] at the VUV wavelength of 500 Å. It also represents the interface between dense glass ($n_0 = 1.66$) and a strongly absorbing aqueous (dye) solution[7] ($n_1 = 1.33 - j0.025$) in the visible or near IR. With the substitution of $\epsilon = 0.64 - j0.024$ into Eqs. (18), the solution of Eq. (16) gives three roots[8]:

$$u_1 = -0.3990,$$
$$u_2 = 0.3902,$$
$$u_3 = 0.5146. \tag{20}$$

From Eq. (17) it is evident that the first root u_1 is physically meaningless and hence can be ignored. u_2 and u_3 are both acceptable and yield angles of incidence

$$\phi_2 = 38.657°,$$
$$\phi_3 = 45.836°. \tag{21}$$

Because $\tan\phi_2 \cong \epsilon_r^{1/2}$, one can correctly infer that ϕ_2 is the angle of minimum $|r_p|$, i.e., the pseudo-Brewster angle. ϕ_3 is a new angle that specifies an extremum, a minimum, of the AIR phase shift function $\delta_p(\phi)$. This is verified by calculating $\mathrm{Re}(r_p'/r_p)^2$ at ϕ_2 and ϕ_3, which turn out to be <0 and >0, respectively.[9] According to the theorem given in Section 2, this indicates that ϕ_2 and ϕ_3 locate extrema of $|r_p|$ and δ_p, respectively. This is demonstrated further in Fig. 1, which is a plot of $|r_p|$ versus ϕ, and Fig. 2, which is a plot of δ_p versus ϕ. As expected, $|r_p|$ has a single minimum at $\phi_2 = 38.657°$; the associated minimum amplitude reflectance is

$$|r_p|_{\min} = 0.0053. \tag{22}$$

Figure 2 shows that δ_p has a minimum of its own at $\phi_3 = 45.836°$; the associated minimum AIR phase shift is

$$\delta_{p_{\min}} = 14.2865°. \tag{23}$$

An excellent approximation to ϕ_3, denoted by ϕ_{3a}, is given by

$$\phi_{3a} = (\phi_B^{\mathrm{nom}} + \phi_C^{\mathrm{nom}})/2$$
$$= (\tan^{-1}\epsilon_r^{1/2} + \sin^{-1}\epsilon_r^{1/2})/2. \tag{24}$$

ϕ_{3a} is the arithmetic mean of the nominal Brewster and critical angles that are obtained when the imaginary part of complex ϵ ($\epsilon_i \ll 1$) is neglected. For the present example, ϵ_r

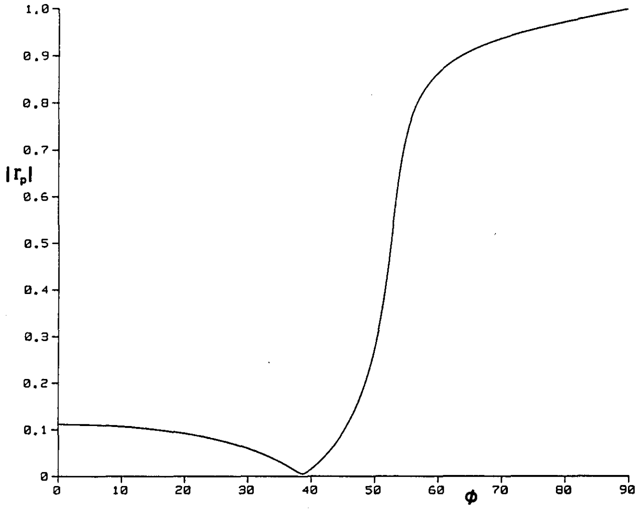

Fig. 1. Amplitude reflectance $|r_p|$ versus the angle of incidence ϕ for AIR of p-polarized light at an interface with complex relative dielectric constant $\epsilon = 0.64 - j0.024$. $|r_p|$ is minimum at the pseudo-Brewster angle $\phi_{pB} = 38.657°$.

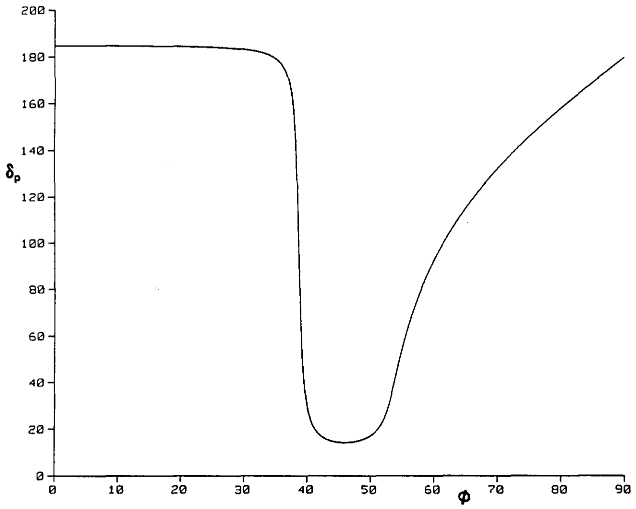

Fig. 2. AIR phase shift for the p polarization δ_p plotted versus the angle of incidence ϕ for an interface with $\epsilon = 0.64 - j0.024$. δ_p goes through a minimum of its own at an angle, $\phi_{\delta p_{\min}} = 45.836°$, that is determined by another root of the same cubic equation of the pseudo-Brewster angle ϕ_{pB}.

= 0.64, and Eq. (24) gives $\phi_{3a} = 45.895°$, which differs from the exact ϕ_3 (at which δ_p is minimum) [Eq. (21)] by ~0.06°. Intuitively, one can state that

$$\lim_{\epsilon_i \to 0} (\phi_3 - \phi_{3a}) = 0 \tag{25}$$

and

$$\lim_{\epsilon_i \to 0} \delta_{p_{\min}} = 0. \tag{26}$$

B. Ratio of Complex *p* and *s* Reflection Coefficients

As another complex function of a real variable, consider the ratio of Fresnel reflection coefficients for the p (TM) and s (TE) polarizations[10]:

$$r_p/r_s = \rho(\phi) = \frac{\sin\phi \tan\phi - (\epsilon - \sin^2\phi)^{1/2}}{\sin\phi \tan\phi + (\epsilon - \sin^2\phi)^{1/2}}, \tag{27}$$

where ϕ is the angle of incidence and ϵ is the complex relative dielectric constant of the reflecting interface, as before. ρ can be written as

$$\rho = |\rho|\exp(j\Delta), \tag{28}$$

where the relative amplitude attenuation $|\rho|(= \tan\psi)$ and the differential reflection phase shift Δ $(= \delta_p - \delta_s)$ are measurable by ellipsometry.[10] From Section 2, the extrema of $|\rho|$ and Δ as functions of ϕ are determined by solving one and the same equation:

$$\text{Im}(\rho'/\rho)^2 = 0. \tag{29}$$

Equations (27) and (29) were shown previously[11] to lead to a quartic equation,

$$\sum_{i=0}^{4} a_i u^i = 0, \tag{30}$$

where $u = \sin^2\phi$, as before, and the coefficients a_i are determined by complex ϵ through somewhat involved expressions that are not repeated here. It was thought that Eq. (30) had only one root in the interval $0 < u < 1$, namely, the root that determines the second Brewster angle, ϕ_{2B}, at which $|\rho|$ is minimum $[\text{Re}(\rho'/\rho)^2 < 0]$. This is indeed the case of external reflection when $|\epsilon| > 1$. On the other hand, examples of AIR $(|\epsilon| < 1)$ in which the Δ-versus-ϕ curve exhibits a minimum and a maximum were shown previously,[12] but no simple way of determining the angular positions of these extrema was known. From the theorem given in Section 2, we now know that these angles are also determined by Eq. (30), from two new acceptable roots of this quartic equation. For illustration, consider an interface with the same complex ϵ given by Eq. (19). Solving Eq. (30) explicitly[13] [or, equivalently, solving Eq. (29) by numerical iteration], we obtain the following three angles:

$$\phi_1 = 38.666°,$$
$$\phi_2 = 47.979°,$$
$$\phi_3 = 61.945°. \tag{31}$$

The sign of $\text{Re}(\rho'/\rho)^2$ is negative at ϕ_1 and positive at ϕ_2 and ϕ_3. Therefore $|\rho|$ has an extremum, a minimum, at ϕ_1. This is evidently the second Brewster angle ϕ_{2B} at which

$$|\rho|(\phi_1) = |\rho|_{\min} = 0.024 \tag{32}$$

and $\Delta = \Delta_1 = 92.037°$ as calculated from Eq. (27).

The pseudo-Brewster and second Brewster angles are 0.01° apart and differ little from the principal angle of Δ = 90° (as can be inferred from Δ_1 and the slope of the $\Delta - \phi$ curve at ϕ_1).

ϕ_2 and ϕ_3 locate extrema of the differential reflection phase shift Δ, namely, a minimum and a maximum:

$$\Delta(\phi_2) = \Delta_{\min} = 6.406°,$$
$$\Delta(\phi_3) = \Delta_{\max} = 25.459°. \tag{33}$$

Direct verification of these results appears in Figs. 3 and 4, which show $|\rho|$ and Δ plotted as functions of ϕ.

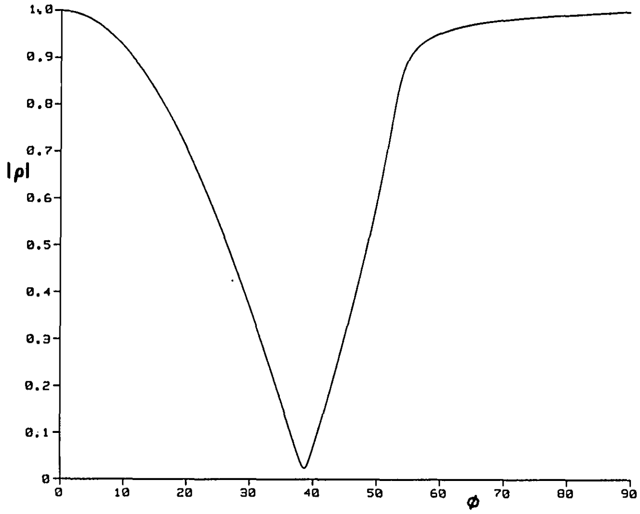

Fig. 3. Ratio of amplitude reflectances for the p and s polarizations $|\rho| = |r_p/r_s|$ plotted versus the angle of incidence ϕ for an interface with $\epsilon = 0.64 - j0.024$. $|\rho|$ is minimum at the second Brewster angle $\phi_{2B} = 38.666°$.

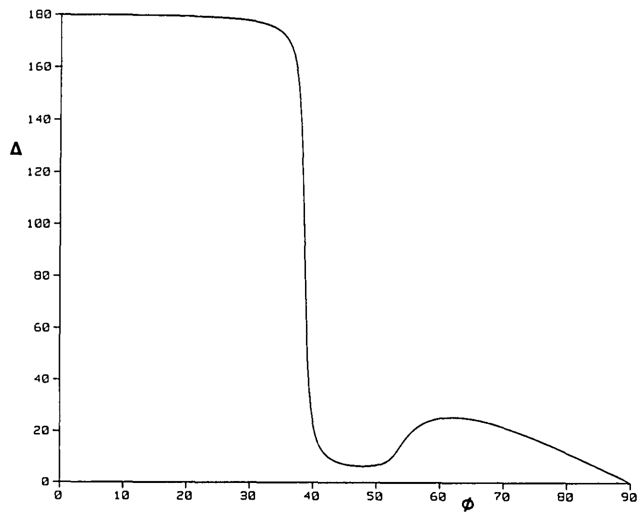

Fig. 4. Difference of the AIR phase shifts for the p and s polarizations $\Delta = \delta_p - \delta_s$ plotted versus the angle of incidence ϕ for an interface with $\epsilon = 0.64 - j0.024$. Δ goes through a minimum and a maximum at angles of incidence $\phi_{\Delta_{\min}} = 47.979°$ and $\phi_{\Delta_{\max}} = 61.945°$, which are determined by two other roots of the same quartic equation that specifies the second Brewster angle ϕ_{2B}.

4. OTHER APPLICATIONS

As another application, consider the reflection at normal incidence (in air, $N_0 = 1$) of a monochromatic plane wave of light by an absorbing substrate of a complex refractive index N_2 coated by a transparent birefringent film of uniform thickness d and principal refractive indices N_{1x} and N_{1y} along two orthogonal principal axes x and y parallel to the film planar boundaries. The principal reflection coefficients of such a system are given by

$$R_\nu = (r_{01\nu} + r_{12\nu}X_\nu)/(1 + r_{01\nu}r_{12\nu}X_\nu), \qquad \nu = x, y, \tag{34}$$

where $r_{ij\nu}$ is the Fresnel reflection coefficient of the ij interface for the ν polarization and

$$X_\nu = \exp(-j4\pi N_{1\nu}\zeta), \qquad \nu = x, y, \tag{35}$$

$$\zeta = d/\lambda. \tag{36}$$

ζ is the normalized film thickness, and λ is the wavelength of light. We are interested in the ratio

$$\rho = R_y/R_x = |\rho|\exp(j\Delta), \tag{37}$$

which is measurable by perpendicular-incidence ellipsometry.[14] In particular, we examine $\rho(\zeta)$ as a complex function of the real argument ζ and look for the extrema of $|\rho|$ and Δ. From Eqs. (34), (35), and (37), we get

$$(\rho'/\rho) = (-j4\pi)\,(U_y - U_x) \tag{38}$$

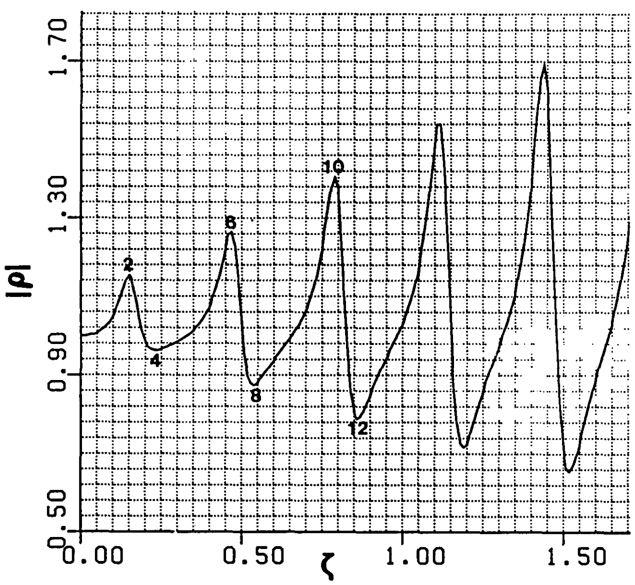

Fig. 5. Ratio of normal-incidence amplitude reflectances for the x and y linear polarizations, $|\rho| = |R_y/R_x|$, parallel to the principal axes of a birefringent film with principal refractive indices $N_{1x} = 1.55$ and $N_{1y} = 1.50$, plotted versus the normalized film thickness $\zeta = d/\lambda$. The birefringent film overlays a Si substrate with a complex refractive index $N_2 = 3.85 - j0.02$ at a wavelength $\lambda = 632.8$ nm.

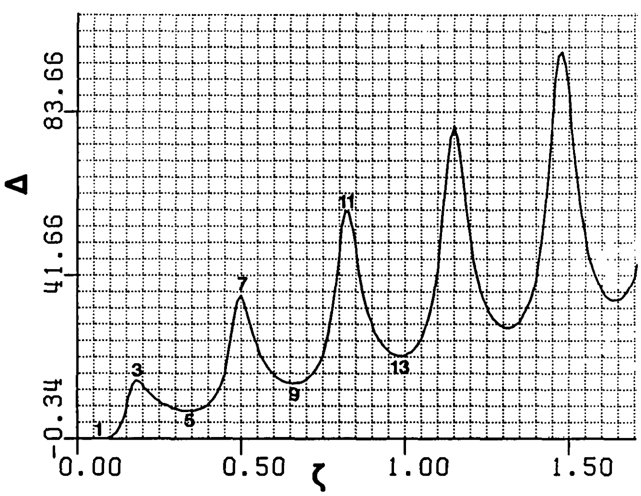

Fig. 6. The differential reflection phase shift $\Delta = \delta_y - \delta_x$ for the same birefringent film on Si as in Fig. 5 (also plotted versus ζ).

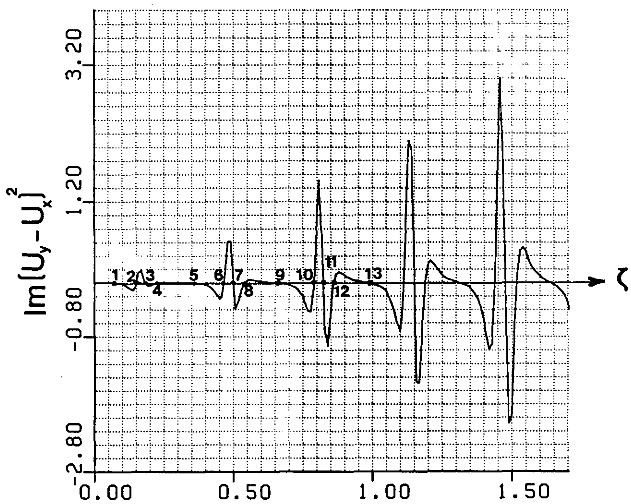

Fig. 7. The function $\mathrm{Im}(U_y - U_x)^2$ plotted versus ζ. Its roots [Eq. (40)], represented by the points of intersection of the curve with the ζ axis, determine the location of the extrema of $|\rho|$ and Δ that appear in Figs. 5 and 6.

Table 1. First 13 Roots of Eq. (40) for a Birefringent Film ($N_{1x} = 1.55$, $N_{1y} = 1.50$) on a Si Substrate ($N_2 = 3.85 - j0.02$) at $\lambda = 632.8$ nm[a]

Root Number	ζ	$\|\rho\|$	Δ (deg)
Odd			
1	0.060208	1.012324	−0.334490 (min)
3	0.183273	1.039571	14.701045 (max)
5	0.340154	1.007657	6.954224 (min)
7	0.499477	1.041112	36.585613 (max)
9	0.661936	1.007624	13.999349 (min)
11	0.824097	1.040670	58.769714 (max)
13	0.987661	1.007764	21.063557 (min)
Even			
2	0.151350	1.156040 (max)	7.984678
4	0.232021	0.963631 (min)	10.693100
6	0.467975	1.269146 (max)	24.173576
8	0.538251	0.876017 (min)	26.417261
10	0.790885	1.406568 (max)	40.041885
12	0.862099	0.790507 (min)	42.281879

[a] The even-numbered roots define the extrema of $|\rho|$, and the odd-numbered ones define the extrema of Δ.

$$U_\nu = N_{1\nu} r_{12\nu} X_\nu [(r_{01\nu} + r_{12\nu} X_\nu)^{-1} - r_{01\nu}(1 + r_{01\nu} r_{12\nu} X_\nu)^{-1}], \quad \nu = x, y, \tag{39}$$

where the prime indicates the first partial derivative with respect to ζ. The extrema of $|\rho|$ and Δ as functions of ζ are determined by $\mathrm{Im}(\rho'/\rho)^2 = 0$ or, equivalently,

$$\mathrm{Im}(U_y - U_x)^2 = 0 \tag{40}$$

and correspond to $\mathrm{Re}(U_y - U_x)^2$ values that are >0 and <0, respectively.

As a specific example, we take a Si substrate with complex refractive index $N_2 = 3.85 - j0.02$ at $\lambda = 632.8$ nm. For the film, we assume that $N_{1x} = 1.55$ and $N_{1y} = 1.50$. Figures 5, 6, and 7 show $|\rho|$, Δ, and $\mathrm{Im}(U_y - U_x)^2$, respectively, plotted as functions of ζ in the range 0–1.5. Both $|\rho|$ and Δ show multiple extrema whose locations are determined by the intersections of the curve of $\mathrm{Im}(U_y - U_x)^2$ with the ζ axis. The first 13 extrema, which occur in the interval $0 < \zeta < 1$, are numbered. The corresponding numerical data, obtained by solution of Eq. (40) and subsequent use of Eqs. (34)–(37), are summarized in Table 1. In the determination of each root, iteration on ζ is stopped when the left-hand side of Eq. (40) is $<10^{-6}$.

It should be evident that the theorem given in Section 2 has general application to the reflection and the transmission of monochromatic light by multilayer-coated surfaces. It applies not only to the complex amplitude reflectance and transmittance considered as functions of frequency, as in the case of spectral filters, but also to these characteristics when they are viewed as functions of the angle of incidence, the layer thicknesses, and the optical properties.

Other applications are anticipated in the physical optics of propagation, interference, scattering, and diffraction. These are, of course, outside the scope of this paper.

APPENDIX A

Instead of the polar form [Eq. (1)] consider the Cartesian form

$$F(\omega) = F_r(\omega) + jF_i(\omega). \tag{A1}$$

Take the first derivative with respect to ω:

$$F'(\omega) = F_r'(\omega) + jF_i'(\omega). \tag{A2}$$

Let

$$H = (F')^2, \tag{A3}$$

so that

$$\mathrm{Re}\, H = (F_r')^2 - (F_i')^2, \tag{A4}$$

$$\mathrm{Im}\, H = 2F_r'F_i'. \tag{A5}$$

The extrema of F_r and F_i as functions of ω are determined simultaneously by solving one and the same equation,

$$\mathrm{Im}[H(\omega)] = 0, \tag{A6}$$

as is apparent from Eq. (A5). The extrema of F_r and F_i are distinguished as follows:

$$\mathrm{Re}\, H < 0 \quad \text{if } F_r' = 0, \tag{A7}$$

$$\mathrm{Im}\, H > 0 \quad \text{if } F_i' = 0. \tag{A8}$$

ACKNOWLEDGMENTS

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