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# Bounds and zeros in reflection and refraction by uniaxial crystals

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Abstract. Bounds are given for the possible values of the following quantities: the reflection amplitudes  $r_{ss}$ ,  $r_{pp}$ ,  $r_{sp}$ ,  $r_{ap}$ , and  $r_{ps}$ ; the transmission amplitudes  $t_{so}$ ,  $t_{se}$ ,  $t_{po}$ ,  $t_{pe}$ ; the Brewster angle given by the zero of  $r_{pp}$ ; and the angle between the extraordinary ray and the extraordinary wavevector. These bounds are for arbitrary orientation of the optic axis relative to the reflecting surface and for any angle of incidence. Index matching enhances the effects of anisotropy, particularly in the reflection properties. For example, the bounds on the Brewster angle approach 0° and 90° as the refractive index of the medium of incidence tends to the lower of the ordinary and extraordinary refractive indices. A formula is given for the Brewster angle in the case where the optic axis lies in the plane of incidence. The conditions under which the four transmission amplitudes can be zero are also discussed.

#### 1. Introduction

The purpose of this note is to present limits on the reflection and refraction properties of uniaxial crystals. Although bounds on the optical properties of crystals (as a function of the crystal orientation, for example) are of practical and theoretical importance, there seems to be no discussion of such in the optical texts (see for example [1-3]). We will use the analytical results recently obtained for this problem [4]. As in [4], the reflecting surface is in the x-y-plane, and the plane of incidence is the z-x-plane, with the z-axis directed normally into the crystal. The medium of incidence has refractive index  $n_1$ , the crystal is characterized by ordinary and extraordinary refractive indices  $n_0$  and  $n_e$ , and the angle of incidence is  $\theta$ . The optic axis c has direction cosines  $\alpha$ ,  $\beta$  and  $\gamma$  with the x-, y- and z-axes, with  $\alpha^2+\beta^2+\gamma^2=1$ , so that c is the unit vector

$$c = (\alpha, \beta, \gamma) \tag{1}$$

In the reflection-refraction problem, the tangential component of the wavevector is the same for the incident, reflected and refracted waves, and is written as

$$K = \left(\frac{\omega}{c}\right) n_1 \sin \theta. \tag{2}$$

The normal components of the wavevector are respectively  $q_1$ ,  $-q_1$ ,  $q_0$  and  $q_e$  for the incident, reflected, and refracted ordinary and extraordinary waves. The values of  $q_1$  and  $q_0$  are given by

$$q_1^2 = \epsilon_1 \omega^2 / c^2 - K^2$$
  $q_0^2 = \epsilon_0 \omega^2 / c^2 - K^2$  (3)

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where  $\epsilon_1 = n_1^2$  is the dielectric constant of the medium of incidence, and  $\epsilon_0 = n_0^2$  ( $n_0$  and  $n_e$  are the ordinary and extraordinary refractive indices). In contrast to  $q_0$ ,  $q_e$  depends on the orientation of the optic axis:

$$q_{\rm e} = [[n_0 \{\epsilon_{\rm e} \epsilon_{\gamma} \omega^2 / c^2 - (\epsilon_{\rm e} - \beta^2 \Delta \epsilon) K^2 \}^{1/2} - \alpha \gamma K \Delta \epsilon]] / \epsilon_{\gamma}$$
<sup>(4)</sup>

where  $\epsilon_e = n_e^2$ ,  $\Delta \epsilon = \epsilon_e - \epsilon_o$ , and  $\epsilon_e = n_e^2 - \epsilon_e \pm \gamma^2$ 

$$\epsilon_{\gamma} = n_{\gamma}^2 = \epsilon_0 + \gamma^2 \Delta \epsilon.$$
<sup>(5)</sup>

Bounds on  $q_e$  were established in [4], where it was shown that  $q_e^2$  is bounded by  $q_o^2$  and by

$$u_{\rm m}^2 = \epsilon_{\rm e} \omega^2 / c^2 - K^2. \tag{6}$$

The  $q_o^2$  bound is attained when  $\beta = 0$  (optic axis in plane of incidence) and  $\alpha q_o = \pm \gamma K$ . The  $q_m^2$  value is attained when  $\beta^2 = 1$  (and  $\alpha, \gamma = 0$ ), the optic axis then being perpendicular to the plane of incidence, and also when  $\alpha K + \gamma q_e = 0$ . As noted in [4], when  $\alpha K + \gamma q_e = 0$  (wavevector  $k_e \equiv (K, 0, q_e)$  is perpendicular to the optic axis) the extraordinary wavevector and ray directions are both that of  $(\gamma, 0, -\alpha)$ , and are thus perpendicular to the optic axis ( $\alpha, \beta, \gamma$ ). Also  $E_e$  is then parallel to the optic axis. Since  $E_o$  is always perpendicular to the optic axis (see equation (7) below), the ordinary and extraordinary electric fields are orthogonal in this configuration. The requirements on the direction cosines are  $\alpha \gamma < 0$ ,  $\gamma^2 \epsilon_e < (\alpha^2 + \gamma^2) \epsilon_1$ . For given  $\alpha$  and  $\gamma$  satisfying the above conditions, the angle of incidence is given by  $n_1 \sin \theta = n_e \{\gamma^2/(\alpha^2 + \gamma^2)\}^{1/2}$ , which shows that Snell's law is obeyed by the extraordinary ray (and wavevector) in this case.

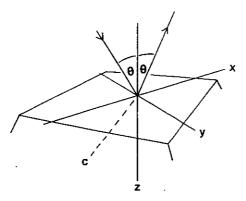


Figure 1. Reflection from a crystal face. The z-axis is the inward normal, the z-x-plane is the plane of incidence, and the angle of incidence is  $\theta$ . The refracted wave directions are not shown. The optic axis c is shown by the broken line. It is specified by direction cosines  $\alpha$ ,  $\beta$  and  $\gamma$ : for example  $\gamma$  is the cosine of the angle between c and the z-axis.

The ordinary and extraordinary electric field vectors are given by

$$E_{o} = N_{o}(-\beta q_{o}, \alpha q_{o} - \gamma K, \beta K)$$

$$E_{e} = N_{e}(\alpha q_{o}^{2} - \gamma q_{e}K, \beta \epsilon_{o} \omega^{2}/c^{2}, \gamma(\epsilon_{o} \omega^{2}/c^{2} - q_{e}^{2}) - \alpha q_{e}K).$$
(7)

 $N_o$  and  $N_e$  are normalization factors. A convenient normalization is to unit magnitude, i.e. so that  $E_o^2$  and  $E_e^2$  are both unity. Note that  $E_o$  is always orthogonal to the optic axis, and also to the ordinary wavevector  $(K,0,q_o)$ .

## 2. Bounds on the reflection amplitudes and on the Brewster angle

We begin with  $r_{ss}$ , which gives the amplitude reflected into the s polarization when the incident wave is s polarized. From equations (34) and (35) of [4] we find that  $r_{ss}$  can be written in the form

$$r_{\rm ss} = (a(q_1 - q_{\rm o}) + b(q_1 - q_{\rm e})) / (a(q_1 + q_{\rm o}) + b(q_1 + q_{\rm e}))$$
(8)

where

$$a = (\alpha q_{o} - \gamma K) \{ \alpha (k_{o}^{2} q_{e} + q_{1} q_{o}^{2}) - \gamma K (k_{o}^{2} - q_{t} q_{e}) \} \qquad b = \beta^{2} k_{o}^{2} (k_{o}^{2} + q_{t} q_{o})$$

$$q_{t} = q_{1} + K \tan \theta = k_{1}^{2} / q_{1} \qquad k_{o}^{2} = \epsilon_{o} \omega^{2} / c^{2} \qquad k_{1}^{2} = \epsilon_{1} \omega^{2} / c^{2}.$$
(9)

When the optic axis lies in the plane of incidence,  $r_{ss}$  reduces to

$$r_{\rm ss}(\beta = 0) = (q_1 - q_0)/(q_1 + q_0) \tag{10}$$

When the optic axis is perpendicular to the plane of incidence,  $r_{ss}$  reduces to

$$r_{\rm ss}(\beta^2 = 1) = (q_1 - q_{\rm m})/(q_1 + q_{\rm m}). \tag{11}$$

The two expressions (10) and (11) are bounds on  $r_{ss}$  (see figure 2). When  $\epsilon_o > \epsilon_e$ the  $\beta = 0$  value is the upper bound and the  $\beta^2 = 1$  value is the lower bound. Note that (10) and (11) are of the form  $(q_1 - q_2)/(q_1 + q_2)$ , which is the s polarization Fresnel amplitude for reflection at a boundary between isotropic media of refractive indices  $n_1$  and  $n_2$  (see for example [1] section 1.5.2, or [5] section 1-1). That bounds on  $r_{ss}$  are attained in configurations where the optic axis lies parallel and perpendicular to the plane of incidence is in accord with physical expectation, given that  $E_o$  is always normal to the optic axis, and the electric vector of the incident s wave is normal to the plane of incidence.

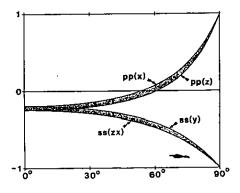


Figure 2. Reflection amplitudes  $r_{15}$  and  $r_{pp}$ , as functions of the angle of incidence, drawn for calcite ( $n_0 = 1.658$ ,  $n_e = 1.486$ ) in air. The full curves are the bounds of equations (10), (11), (15) and (16), with x, y, z or zx indicating that the optic axis lies along the x, y or z axes, or in the z-x-plane (the plane of incidence). The points are calculated from (8) and (12) with randomly chosen  $\alpha, \beta, \gamma$  and  $\theta$  (uniformly distributed over their range).

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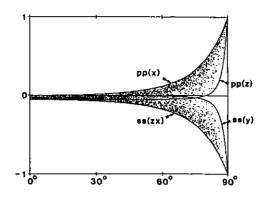


Figure 3. Reflection by calcite in castor oil  $(n_1 = 1.48)$ : the amplitudes  $r_{pp}$  and  $r_{ss}$  are plotted versus the angle of incidence, the curves from equations (10), (11), and (15), (16), the points for random values of  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\theta$ , calculated from (8) and (12).

Next we look at  $r_{pp}$ , the amplitude reflected into the p polarization when the incident wave is p polarized. This is also shown in figure 2. From equation (42) in [4] we find that

$$-r_{pp} = [\beta^{2}k_{o}^{2}(q_{1} + q_{e})(k_{o}^{2} - q_{1}q_{o}) + (q_{1} + q_{o})(\alpha q_{o} - \gamma K)\{\alpha(k_{o}^{2}q_{e} - q_{1}q_{o}^{2}) - \gamma K(k_{o}^{2} - q_{1}q_{e})\}]/[\beta^{2}k_{o}^{2}(q_{1} + q_{e})(k_{o}^{2} + q_{1}q_{o}) + (q_{1} + q_{o})(\alpha q_{o} - \gamma K) \times \{\alpha(k_{o}^{2}q_{e} + q_{1}q_{o}^{2}) - \gamma K(k_{o}^{2} + q_{1}q_{e})\}]$$
(12)

At grazing incidence, where  $q_1 \rightarrow 0$ ,  $r_{pp} \rightarrow 1$ . From (8) we see that  $r_{ss} \rightarrow -1$  at grazing incidence. It is interesting to note that for reflection from arbitrarily stratified isotropic media,  $r_p \rightarrow 1$  and  $r_s \rightarrow -1$  at grazing incidence ([5] section 2-3). For reflection from an isotropic layer on a uniaxial substrate, it is also true that  $r_{pp} \rightarrow 1$  and  $r_{ss} \rightarrow -1$  at grazing incidence ([6] section 4). The cross-reflection amplitudes  $r_{sp}$  and  $r_{ps}$  go to zero at grazing incidence, for a crystal with or without an isotropic overlayer.

When the optic axis lies in the plane of incidence, the expression (12) reduces to

$$r_{\rm pp}(\beta = 0) = (Q_{\gamma} - Q_1) / (Q_{\gamma} + Q_1)$$
(13)

where

$$Q_1 = q_1/\epsilon_1, \qquad Q_\gamma = q_\gamma/n_o n_e \qquad q_\gamma^2 = \epsilon_\gamma \omega^2/c^2 - K^2. \tag{14}$$

Bounds on  $r_{pp}$  may be obtained from geometries which are special cases of  $\beta = 0$ . When the optic axis lies along the intersection of the plane of incidence and the reflecting plane ( $c \parallel x$ ), and with  $Q_e = q_0/n_o n_e$ ,

$$r_{\rm pp}(\alpha^2 = 1) = (Q_{\rm e} - Q_1)/(Q_{\rm e} + Q_1).$$
 (15)

When the optic axis coincides with the surface normal (reflection from a basal plane), we find from equation (51) in [4] that, with  $Q = q_e/\epsilon_o = q_m/n_o n_e$ 

$$r_{\rm pp}(\gamma^2 = 1) = (Q - Q_1)/Q + Q_1)$$
 (16)

where  $q_e$  is given by equation (49) in [4]:

$$q_{\rm e}^2 = \epsilon_{\rm o}(\omega^2/c^2 - K^2/\epsilon_{\rm e}) = (\epsilon_{\rm o}/\epsilon_{\rm e})q_{\rm m}^2. \tag{17}$$

The expressions (13), (15) and (16) are of the form  $(Q_2-Q_1)/(Q_2+Q_1)$ , which is the p polarization Fresnel amplitude for reflection at a boundary between isotropic media with dielectric constants  $\epsilon_1$  and  $\epsilon_2$ , with  $Q_1 = q_1/\epsilon_1$ ,  $Q_2 = q_2/\epsilon_2$  ([1], section 1.5.2; [5] section 1-2). From figure 2 we see that (15) and (16) are bounds for  $r_{pp}$ . When  $\epsilon_0 > \epsilon_e$  the  $\alpha^2 = 1$  value is the upper bound, and the  $\gamma^2 = 1$  value is the lower bound.

For a boundary between isotropic transparent media, the Brewster angle is defined by  $r_p = 0$ , which gives  $\tan \theta_B = n_2/n_1$ . Let us define the Brewster angle for a boundary between an isotropic medium of index  $n_1$  and a uniaxial crystal with indices  $n_0$  and  $n_e$  by  $r_{pp} = 0$ . Then the bounds (10) and (11) also provide bounds on  $\theta_B$ , namely

$$\tan^2 \theta_{\rm B}(\alpha^2 = 1) = [\epsilon_{\rm o}(\epsilon_{\rm e} - \epsilon_{\rm i})] / [\epsilon_{\rm i}(\epsilon_{\rm o} - \epsilon_{\rm i})]$$
(18)

$$\tan^2 \theta_{\rm B}(\gamma^2 = 1) = [\epsilon_{\rm e}(\epsilon_{\rm o} - \epsilon_1)] / [\epsilon_1(\epsilon_{\rm e} - \epsilon_1)]$$
<sup>(19)</sup>

These expressions have been given as equations (62) and (52) in [4], respectively. They are special cases of the following formula, obtained from (13):

$$\tan^2 \theta_{\rm B}(\beta=0) = (\epsilon_{\rm o}\epsilon_{\rm e} - \epsilon_{\rm I}\epsilon_{\gamma})/[\epsilon_{\rm I}(\epsilon_{\gamma} - \epsilon_{\rm I})]. \tag{20}$$

This equation gives the Brewster angle when the optic axis lies in plane of incidence. Note the effect of an index-matching fluid: the range of  $\theta_{\rm B}$  expands to  $(0^{\circ}, 90^{\circ})$  when  $\epsilon_1$  tends to the smaller of  $\epsilon_0$  and  $\epsilon_e$ . This is illustrated in figure 3, which shows the pp and ss reflection amplitudes for calcite in castor oil.

Finally we consider the  $r_{sp}$  and  $r_{ps}$  reflection amplitudes. These give the amount reflected into the p polarization when s polarization is incident, and vice versa. At normal incidence, from equation (73) in [4],

$$r_{\rm sp} = r_{\rm ps} = \frac{2\alpha\beta}{\alpha^2 + \beta^2} \frac{n_1 n_0 (n_\gamma - n_e)}{(n_1 + n_0)(n_1 n_\gamma + n_0 n_e)}.$$
 (21)

The magnitude of the prefactor  $2\alpha\beta/(\alpha^2 + \beta^2)$  is maximized when  $|\alpha| = |\beta|$ , and is then unity. The magnitude of the remaining factor is maximized by  $\gamma = 0$  (the optic axis then lies in the reflecting plane, as in reflection by a prism face of a hexagonal crystal). Thus at normal incidence

$$|r_{\rm sp}|, |r_{\rm ps}| \le (n_1|n_{\rm o} - n_e|) / [(n_1 + n_{\rm o})(n_1 + n_e)]$$
(22)

where the right-hand side is attained when the optic axis is  $c = (\pm 1/\sqrt{2}, \pm 1/\sqrt{2}, 0)$ . The same result follows from [6], equation (19). A fair approximation for the general incidence bound is suggested by (22):

$$|r_{\rm sp}|, |r_{\rm ps}| \lesssim (q_1|q_{\rm o} - q_{\rm m}|) / [(q_1 + q_{\rm o})(q_1 + q_{\rm m})].$$
<sup>(23)</sup>

The maximum of the right side of (23), as a function of the angle of incidence, occurs when  $q_0q_m = q_1(q_1 + q_0 + q_m)$ , which may be reduced to the following quartic in  $y = (cq_1/\omega)^2 = \epsilon_1 \cos^2 \theta$ :

$$y^{4} + 2(u+v)y^{3} + 4uvy^{2} - u^{2}v^{2} = 0$$
(24)

where  $u = (\epsilon_o - \epsilon_1)/2$  and  $v = (\epsilon_e - \epsilon_1)/2$ . The relevant solution of this quartic is  $y = (\sqrt{2} - 1)(u + v)/2 = (\sqrt{2} - 1)(\epsilon_o + \epsilon_e - 2\epsilon_1)/4$ , plus terms of even order in  $\Delta \epsilon = \epsilon_e - \epsilon_o$ . Thus a maximum occurs at an angle given approximately by

$$\cos^2\theta \approx (\sqrt{2} - 1)(\epsilon_o + \epsilon_e - 2\epsilon_1)/4\epsilon_1 \tag{25}$$

The value of the right-hand side of (23) at this angle, to lowest order in  $\Delta \epsilon / (\epsilon_0 + \epsilon_e - 2\epsilon_1)$ , is

$$|\Delta \epsilon| / [(\sqrt{2} - 1)^2 (\epsilon_{o} + \epsilon_{e} - 2\epsilon_{1})].$$
<sup>(26)</sup>

This expression suggests that index-matching enhances the cross-reflection amplitudes, as is indeed the case.

The general form of the s-to-p and p-to-s reflection amplitudes is, from equation (47) of [4],

$$r_{\rm sp}, r_{\rm ps} = 2\beta(\alpha q_{\rm o} \pm \gamma K)(q_{\rm o} - q_{\rm e})k_1k_o^2/[a(q_1 + q_{\rm o}) + b(q_1 + q_{\rm e})]$$
(27)

the upper sign applying to  $r_{\rm sp}$ , the lower to  $r_{\rm ps}$ . A better approximation than (23) to the bound on  $|r_{\rm sp}|$  and  $|r_{\rm ps}|$  is obtained by calculating  $r_{\rm ps}$  in the special configuration where  $\beta^2 = 1/2$  and  $\alpha K + \gamma q_e = 0$ . The latter condition, discussed in [4] following equation (29), makes  $E_e$  parallel to c (also the extraordinary wavevector and ray direction are the same, and perpendicular to the optic axis). When  $\alpha K + \gamma q_e = 0$ we have from equation (22) in [4]

$$\alpha^2 K^2 = \gamma^2 q_{\rm m}^2 \qquad q_{\rm e}^2 = q_{\rm m}^2.$$
 (28)

If in addition  $\beta^2 = \frac{1}{2}$ , the values of  $\alpha^2$  and  $\gamma^2$  are fixed when the angle of incidence is specified:

$$\alpha^2 = (cq_{\rm m}/\omega)^2/(2\epsilon_{\rm e}) \qquad \gamma^2 = (cK/\omega)^2/(2\epsilon_{\rm e}) \tag{29}$$

and the p-to-s reflection amplitude becomes

$$r_{\rm ps}^{\rm m} = \frac{2 {\rm sgn}(\alpha\beta) n_1 n_e q_1 (q_{\rm o} - q_{\rm m}) (q_{\rm o} q_{\rm m} + K^2)}{(q_1 + q_{\rm o}) \{2 \epsilon_{\rm e} q_{\rm o} (q_1 q_{\rm m} + \epsilon_1 \omega^2 / c^2) + K^2 [\epsilon_{\rm e} (2q_1 + q_{\rm m} - q_{\rm o}) + \epsilon_1 (q_{\rm m} - q_{\rm o})]\}}$$
(30)

This expression provides an approximation to the bounds on  $r_{ps}$  and  $r_{sp}$ , as shown in figure 4.

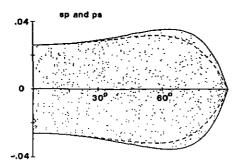


Figure 4. The cross reflection amplitudes  $r_{ps}$  and  $r_{sp}$ , for calculate in air. The points are for randomly chosen angles of incidence and optic axis orientation, the curves are approximate bounds from equations (23) and (30) (dashed and full curves, respectively).

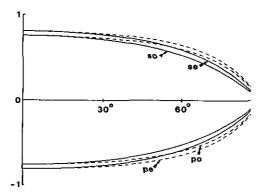


Figure 5. Bounds for the transmission amplitudes  $t_{sc}$ ,  $t_{so}$ ,  $t_{pe}$ ,  $t_{po}$  as a function of the angle of incidence, for calcite in air. The solid curves are bounds on  $t_{se}$  and  $t_{so}$  (equations (37) and (38)); the dashed curves are approximate bounds on  $t_{po}$  and  $t_{pe}$  (expressions (41) and (45)).

## 3. Bounds on transmission properties

We shall first discuss zeros and bounds of the transmission amplitudes  $t_{so}$ ,  $t_{se}$ ,  $t_{po}$ ,  $t_{pe}$ , and then give a bound on the angle between the extraordinary ray and wavevector. The transmission amplitudes are particularly simple at normal incidence (see [4], equations (78) and (79). From these we find that

$$|t_{so}|, |t_{po}| \le 2n_1/(n_1 + n_o) \tag{31}$$

$$|t_{\rm se}|, |t_{\rm pe}| \le 2n_1/(n_1 + n_l) \tag{32}$$

where  $n_i$  is the lesser of  $n_o$  and  $n_e$ . For comparison, we note that the transmission amplitude at normal incidence into an isotropic medium of index  $n_2$  is  $2n_1/(n_1+n_2)$ . The bound (31) on  $t_{so}$  and  $t_{po}$  follows by inspection of equations (78) and (79) in [4]. The bound on  $t_{se}$  is obtained as follows: it is clear from equation (78) in [4] that the magnitude of  $t_{se}$  is largest when  $\alpha = 0$ . With the use of equation (77) in [4],  $t_{se}(\alpha = 0)$  reduces to

$$t_{\rm se} = \operatorname{sgn}(\beta) [(\epsilon_{\rm o} + \epsilon_{\rm e})\epsilon_{\gamma} - \epsilon_{\rm o}\epsilon_{\rm e}]^{1/2} / (\epsilon_{\gamma} + nn_{\gamma})$$
(33)

where  $n = n_o n_e/n_1$ . Setting the derivative of  $t_{se}^2$  with respect to  $n_\gamma$  equal to zero leads to a cubic in  $n_\gamma$ , namely  $\epsilon_o \epsilon_e (n + 2n_\gamma) - (\epsilon_o + \epsilon_e) n_\gamma^3 = 0$ , which has one real root provided  $\epsilon_o + \epsilon_e > \frac{32}{27} \epsilon_1$ . As  $\gamma^2$  varies from 0 to 1, the cubic expression does not change sign provided  $\epsilon_o < \epsilon_e (1 + n_e/n_1)$  and  $\epsilon_e < \epsilon_o (1 + n_o/n_1)$ . When these conditions are satisfied (which is the usual case) the maximum of  $t_{se}^2$  is thus obtained by the greater of the  $\gamma = 0$  and  $\gamma = \pm 1$  values. This gives the bound (32). The case of  $t_{pe}$  is similar, with  $\beta = 0$  giving the largest magnitude, and leading to the same bound subject to the same conditions. (The same results follow by maximizing  $t_e$  as given in equation (20) of [6]).

At general incidence a clue to the maximum of  $|t_{so}|$  is provided by the zero of  $t_{se}$ , and vice versa. From equation (34) of [4] we find (correcting the misprinted sign of  $t_{se}$ ,

$$t_{\rm so} = 2q_1 N_{\rm o}^{-1} [\alpha (k_{\rm o}^2 q_{\rm e} + q_{\rm t} q_{\rm o}^2) - \gamma K(k_{\rm o}^2 + q_{\rm t} q_{\rm e})] / [a(q_1 + q_{\rm o}) + b(q_1 + q_{\rm e})]$$
(34)

$$t_{\rm se} = 2q_1 N_{\rm e}^{-1} \beta (k_{\rm o}^2 + q_1 q_{\rm o}) / [a(q_1 + q_o) + b(q_1 + q_{\rm e})].$$
(35)

We see that  $t_{so}$  is zero when  $\beta^2 = 1$  (optic axis perpendicular to the plane of incidence) and so expect the maximum of  $|t_{se}|$  to occur for that configuration. When  $\beta^2 = 1$  we have  $q_e = q_m$ , and

$$|t_{\rm se}(\beta^2 = 1)| = 2q_1/(q_1 + q_{\rm m}). \tag{36}$$

This expression provides the correct bound when  $\epsilon_e < \epsilon_o$  (as for calcite). The general bound appears to be

$$|t_{se}| \leqslant 2q_1/(q_1+q_i) \tag{37}$$

where  $q_l$  is the lesser of  $q_o$  and  $q_m$ . Conversely, we see that  $t_{se}$  is zero when  $\beta = 0$ , and so expect  $t_{so}$  to have maximum magnitude when the optic axis lies in the plane of incidence. The values of  $t_{so}$  when  $\alpha^2 = 1$  or  $\gamma^2 = 1$  provide the upper bound for  $|t_{so}|$ :

$$|t_{so}| \leq 2q_1/(q_1 + q_0) = |t_{so}(\alpha^2 = 1)| = |t_{so}(\gamma^2 = 1)|.$$
(38)

We now turn to  $t_{po}$  and  $t_{pe}$ . From equation (42) in [4] these are

$$t_{\rm po} = -2k_1 N_{\rm o}^{-1}(q_1 + q_e)\beta k_{\rm o}^2 / [a(q_1 + q_o) + b(q_1 + q_e)]$$
(39)

$$t_{\rm pe} = 2k_1 N_e^{-1} (q_1 + q_0) (\alpha q_0 - \gamma K) / [a(q_1 + q_0) + b(q_1 + q_e)]$$
(40)

Note that  $t_{so}$  and  $t_{pe}$  can pass through zero as the angle of incidence increases, while  $t_{se}$  and  $t_{po}$  keep the same sign. Since  $t_{pe}$  is zero when  $\alpha q_o - \gamma K$  is zero, we expect the maximum of  $|t_{po}|$  to occur when this condition is satisfied, as for example when  $\beta^2 = 1$ . In this configuration (optic axis perpendicular to the plane of incidence) we find

$$|t_{\rm po}(\beta^2 = 1)| = [2Q_1/(Q_1 + Q_o)](n_1/n_o) \qquad Q_o = q_o/\epsilon_o.$$
(41)

This expression is not an exact bound for  $|t_{po}|$ , but is a very good approximation to it. The last transmission amplitude,  $t_{pe}$ , is expected to have maximum magnitude when

 $\beta = 0$ , since this makes  $t_{\rm m}$  zero. Also, the incident p-polarized electric field vector lies in the plane of incidence, and  $|t_{\rm re}|$  should be a maximum when the transmitted extraordinary electric field vector also lies in this plane, which happens when  $\beta = 0$ . For this configuration we find, from (40).

$$t_{\rm pe}(\beta=0) = \frac{2k_1\{(\alpha q_{\rm o}^2 - \gamma q_{\rm e}K^2) + [\gamma (k_{\rm o}^2 - q_{\rm e}^2) - \alpha q_{\rm e}K^2]\}^{1/2}}{\alpha (k_{\rm o}^2 q_{\rm e} + q_{\rm t}q_{\rm o}^2 - \gamma K(k_{\rm o}^2 + q_{\rm t}q_{\rm e}))}.$$
 (42)

When  $\beta = 0$  we have from equations (23) and (24) of [4] that

$$\epsilon_{\gamma}q_{e} = n_{o}n_{e}q_{\gamma} - \alpha\gamma K\Delta\epsilon \tag{43}$$

and this enables a reduction of (42) to

$$t_{\rm pe}^{2}(\beta=0) = 4k_{\rm l}^{2}[\epsilon_{\gamma}^{2}q_{\gamma}^{2} + (n_{\rm o}n_{\rm e}K + \alpha\gamma q_{\gamma}\,\Delta\epsilon)^{2}]/[\epsilon_{\gamma}^{2}(n_{\rm o}n_{\rm e}\omega^{2}/c^{2} + q_{\rm t}q_{\gamma})^{2}]. \tag{44}$$

I have not found an analytic expression for the maximum value of (44). An expression which approximates well the bound of  $|t_{re}|$  is

$$[2Q_1/(Q_1 + Q_l)](n_1/n_l) \qquad Q_l = q_l/\epsilon_l$$
(45)

where  $\epsilon_l$  is the lesser of  $\epsilon_o$  and  $\epsilon_e$ , and  $q_l^2 = \epsilon_l \omega^2 / c^2 - K^2$ . The bounds on the transmission amplitudes are shown in figure 5.

We summarize the conditions under which the transmission amplitudes are zero or maximal:

(i)  $t_{se}$  zero when  $\beta = 0$ ,  $|t_{se}|$  maximum when  $\beta^2 = 1$ ; (ii)  $t_{so}$  zero when  $\alpha(k_o^2 q_e + q_1 q_o^2) = \gamma K(k_o^2 + q_1 q_e), |t_{so}|$  maximum when  $\alpha^2 = 1$ or  $\gamma^2 = 1$ :

(iii)  $t_{pe}$  zero when  $\alpha q_0 = \gamma K$ ,  $|t_{pe}|$  maximum when  $\beta = 0$ ;

(iv)  $t_{po}$  zero when  $\beta = 0$ ,  $|t_{po}|$  maximum when  $\beta^2 = 1$ .

The final transmission property we mention is the angle between the extraordinary ray r and wavevector  $k_e$ . The extraordinary wavevector is  $(K, 0, q_e)$ , and the ray direction is given in [4], equation (31). In section 5.4 of [4] we found that at normal incidence the greatest angle between r and  $k_e$  is  $\delta = \arctan(|\Delta \epsilon|/2n_e n_e)$ . It is remarkable that this same bound appears to be valid at all angles of incidence. However, the angle between r and  $k_0 = (K, 0, q_0)$  is bounded by a curve rather than a constant. The bounding curve increases from  $\delta$  at normal incidence to a larger value at grazing incidence, this value being increased by index matching.

### 4. Discussion

The bounds given in this paper have been obtained by a mixture of physical argument, analysis and numerical trial. Some are explicitly labelled approximate, others are believed to be exact, but a rigorous proof for all possible values of the physical parameters has not been found. Thus, from the strict mathematical viewpoint, they are merely conjectured bounds, which are being presented here in the belief that they may prove useful nevertheless.

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