Variational theory of the reflection of light by interfaces

John Lekner

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

Received February 19, 1985; accepted July 15, 1985

Schwinger's variational theory of scattering is adapted to the calculation of reflection amplitudes. For an arbitrary transition between two media at a planar interface, we derive variational expressions for the s and p reflection amplitudes that are correct at grazing incidence and correct to second order in the ratio of interface thickness to wavelength. The interface or the substrate (or both) may be absorbing. The Hulthén–Kohn variational theory of scattering is also adapted to reflection. The results are simpler (for the same trial wave function) but not so good as those obtained from the Schwinger method.

1. INTRODUCTION

In a previous paper (Ref. 1, referred to here as I) we have derived variational expressions for the reflection amplitudes for a nonuniform film between like media, for example, a soap film in air. Here we shall extend these results to reflection of electromagnetic waves at an interface between any two media of dielectric constants ϵ_1 and ϵ_2. Many of the results of paper I can be carried over to the present work, and in such cases the results will be quoted as [I (equation number)]. In other cases the $\epsilon_1 \neq \epsilon_2$ problem requires special techniques (for example, the Green functions have six analytic parts, instead of just two); then the techniques will be developed in more detail. Where possible the notation used here will be that of I.

2. s-WAVE REFLECTION AMPLITUDE

We consider the problem of plane electromagnetic waves incident from a medium of dielectric constant ϵ_1 onto an interface lying in the xy plane and characterized by a dielectric function $\epsilon(z)$. The medium beyond the interface (the substrate) has dielectric constant ϵ_2. When the propagation is in the zx plane, the s wave has electric field $E = (0, E_y, 0)$, where [I (4)]

$$E_y(z, x) = \exp(iKx)\, E(z) \tag{1}$$

and $E(z)$ satisfies the ordinary differential equation [I (5)]

$$\frac{\mathrm{d}^2E}{\mathrm{d}z^2} + q^2E = 0, \qquad q^2(z) = \epsilon(z)\frac{\omega^2}{c^2} - K^2. \tag{2}$$

The separation of variables constant K is the component of the wave vector along the interface. Thus

$$K = \sqrt{\epsilon_1}\,\frac{\omega}{c}\sin\theta_1 = \sqrt{\epsilon_2}\,\frac{\omega}{c}\sin\theta_2, \tag{3}$$

where θ_1 and θ_2 are the angles of incidence and refraction. The component of the wave number perpendicular to the interface is $q(z)$, and it takes the limiting values

$$\sqrt{\epsilon_1}\,\frac{\omega}{c}\cos\theta_1 = q_1 \leftarrow q(z) \rightarrow q_2 = \sqrt{\epsilon_2}\,\frac{\omega}{c}\cos\theta_2. \tag{4}$$

The reflection amplitude r_s and transmission amplitude t_s are defined in terms of the asymptotic forms of the solution of Eq. (2):

$$\exp(iqz) + r_s\exp(-iqz) \leftarrow E(z) \rightarrow t_s\exp(iqz). \tag{5}$$

It is possible to construct a perturbation theory[2] for r_s in terms of

$$E_0(z) = \begin{cases}\exp(iq_1z) + r_{s0}\exp(-iq_1z) & (z<0)\\ t_{s0}\exp(iq_2z) & (z>0)\end{cases}. \tag{6}$$

Here r_{s0} and t_{s0} are the Fresnel reflection amplitudes[3,4] for the discontinuous (or step) dielectric-function profile

$$\epsilon_0(z) = \begin{cases}\epsilon_1 & (z<0)\\ \epsilon_2 & (z>0)\end{cases}, \tag{7}$$

$$r_{s0} = \frac{q_1 - q_2}{q_1 + q_2}, \qquad t_{s0} = \frac{2q_1}{q_1 + q_2}. \tag{8}$$

$E_0(z)$ is the solution of

$$\frac{\mathrm{d}^2E_0}{\mathrm{d}z^2} + q_0{}^2E_0 = 0, \qquad q_0{}^2(z) = \epsilon_0(z)\frac{\omega^2}{c^2} - K^2 \tag{9}$$

with the correct asymptotic forms for a wave incident from medium one. One constructs a Green function satisfying

$$\frac{\partial^2G}{\partial z^2} + q_0{}^2G = \delta(z - \zeta). \tag{10}$$

This is given by[4]

$$G_s(z, \zeta) = \begin{cases}
\dfrac{E_+(\zeta)[E_-(z) - r_{s0}E_+(z)]}{2iq_2} & (\zeta > z > 0)\\[2mm]
\dfrac{E_+(z)[E_-(\zeta) - r_{s0}E_+(\zeta)]}{2iq_2} & (z > \zeta > 0)\\[2mm]
\dfrac{E_+(\zeta)E_-(z)}{i(q_1 + q_2)} & (z < 0 < \zeta)\\[2mm]
\dfrac{E_+(z)E_-(\zeta)}{i(q_1 + q_2)} & (\zeta < 0 < z)\\[2mm]
\dfrac{E_-(z)[E_+(\zeta) + r_{s0}E_-(\zeta)]}{2iq_1} & (z < \zeta < 0)\\[2mm]
\dfrac{E_-(\zeta)[E_+(z) + r_{s0}E_-(z)]}{2iq_1} & (\zeta < z < 0)
\end{cases} \tag{11}$$

where $E_\pm(z) = \exp(\pm iq_0z)$.

The equation for E can be written as

$$\frac{\mathrm{d}^2E}{\mathrm{d}z^2} + q_0{}^2E = -\Delta q^2E, \tag{12}$$

where $\Delta q^2 = q^2 - q_0{}^2 = \omega^2/c^2(\epsilon - \epsilon_0)$. From Eqs. (9), (10), and (12) we see that E satisfies the integral equation

$$E(z) = E_0(z) - \int_{-\infty}^{\infty} \mathrm{d}\zeta\Delta q^2(\zeta)E(\zeta)G(z, \zeta). \tag{13}$$

The asymptotic form of E as $z \to -\infty$ is found from Eqs. (11) and (13) to be

$$\exp(iq_1z) + \exp(-iq_1 z) \times\left[r_{s0} - \frac{1}{2iq_1}\int_{-\infty}^{\infty} \mathrm{d}\zeta\Delta q^2(\zeta)E(\zeta)E_0(\zeta)\right]\cdot \tag{14}$$

Comparison with Eq. (5) shows that the expression inside the square brackets is the exact value of r_s (this exact result can also be obtained from a comparison identity[4]). The first-order perturbation result is obtained from the exact result on replacing E by E_0 [given by Eq. (6)]:

$$r_s{}^{\text{pert}} = r_{s0} - \frac{1}{2iq_1}\int_{-\infty}^{\infty} \mathrm{d}\zeta\Delta q^2(\zeta)E_0{}^2(\zeta). \tag{15}$$

The adaptation of Schwinger's variational method for the scattering problem[5,6] to the reflection problem runs as follows. We multiply the integral Eq. (13) by $\Delta q^2(z)E(z)$ and integrate over all z. The resulting equation can be put in the form [cf. I (15)] $F = S$, where

$$F = \int_{-\infty}^{\infty} \mathrm{d}z\Delta q^2(z)E(z)E_0(z) \tag{16}$$

is of first degree in the unknown E and

$$S = \int_{-\infty}^{\infty} \mathrm{d}z\Delta q^2(z)E^2(z) + \int_{-\infty}^{\infty} \mathrm{d}z\Delta q^2(z)E(z)\int_{-\infty}^{\infty} \mathrm{d}\zeta\Delta q^2(\zeta)E(\zeta)G(z, \zeta) \tag{17}$$

is of second degree in E. We note that [cf. I (17)]

$$r_s = r_{s0} - F/2iq_1. \tag{18}$$

The variational principle for r_s follows from the result (established in I) that $\delta S = 2\delta F$ or $\delta(F^2/S) = 0$. Thus

$$r_s{}^{\text{var}} = r_{s0} - \frac{F^2/S}{2iq_1}\cdot \tag{19}$$

The simplest variational trial function for $E(z)$ is $E_0(z)$. This gives the values F_0 and S_0 for F and S, where

$$F_0 = \int_{-\infty}^{\infty} \mathrm{d}z\Delta q^2(z)E_0{}^2(z) = -2iq_1(r_s{}^{\text{pert}} - r_{s0}) \tag{20}$$

and

$$S_0 = F_0 + \int_{-\infty}^{\infty} \mathrm{d}z\Delta q^2(z)E_0(z)\int_{-\infty}^{\infty} \mathrm{d}\zeta\Delta q^2(\zeta)E_0(\zeta)G(z, \zeta). \tag{21}$$

The corresponding variational estimate for r_s is [using Eq. (20)]

$$\Delta r_s{}^{\text{var}} = \frac{F_0}{S_0}\Delta r_s{}^{\text{pert}}, \tag{22}$$

where we have introduced the notation $\Delta r = r - r_0$ (in parallel with $\Delta q^2 = q^2 - q_0{}^2$).

This simplest variational result already has built into it two important properties:

(1) To second order in the interface thickness, Eq. (22) gives

$$\Delta r_s{}^{\text{var}} = \frac{2iq_1\omega^2/c^2}{(q_1 + q_2)^2}\left(\lambda_1 + 2iq_2\lambda_2 + \frac{i\omega^2/c^2}{q_1 + q_2}\lambda_1{}^2 + \ldots\right), \tag{23}$$

where[7]

$$\lambda_n = \int_{-\infty}^{\infty} \mathrm{d}z(\epsilon - \epsilon_0)z^{n-1}\cdot \tag{24}$$

This is the correct expression to this order to the interface-thickness–wavelength expansion [see Ref. 7, Eqs. (2) and (15)].

(2) At grazing incidence, when $q_1 \to 0$, $\Delta r_s{}^{\text{var}} \to 0$ when $\epsilon_1 \neq \epsilon_2$, and $\Delta r_s{}^{\text{var}} \to -1$ when $\epsilon_1 = \epsilon_2$. Thus $r_s{}^{\text{var}}$ correctly tends to -1 at grazing incidence, as it must for all interfacial profiles.[8] In contrast, the perturbation expression is in general correct only to first order in the interface thickness and *diverges* at grazing incidence when $\epsilon_1 = \epsilon_2$.

3. p-WAVE REFLECTION AMPLITUDE

For propagation in the zx plane and the interface lying in the xy plane, the p wave has $B = (0, B_y, 0)$, with

$$B_y(z, x) = \exp(iKx)B(z), \tag{25}$$

where K has the same meaning as for the s wave. B satisfies [cf. I (30)]

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon}\frac{\mathrm{d}B}{\mathrm{d}z}\right) + \left(\frac{\omega^2}{c^2} - \frac{K^2}{\epsilon}\right)B = 0, \tag{26}$$

with asymptotic forms[8]

$$\exp(iq_1z) - r_p\exp(-iq_1z) \leftarrow B(z) \rightarrow \sqrt{\frac{\epsilon_2}{\epsilon_1}}\,t_p\exp(iq_2z). \tag{27}$$

The required Green function satisfies

$$\frac{\partial}{\partial z}\left(\frac{1}{\epsilon_0}\frac{\partial G}{\partial z}\right) + \left(\frac{w^2}{c^2} - \frac{K^2}{\epsilon_0}\right)G = \delta(z - \zeta) \tag{28}$$

and is given by[9] [with $B_\pm(z) = \exp(\pm iq_0z)$]

$$G_p(z, \zeta) = \begin{array}{c|c} & \zeta \\ & \dfrac{B_+(\zeta)[B_-(z) + r_{p0}B_+(z)]}{2iQ_2} \quad \zeta = z \\ \dfrac{B_+(\zeta)B_-(z)}{i(Q_1 + Q_2)} & \dfrac{B_+(z)[B_-(\zeta) + r_{p0}B_+(\zeta)]}{2iQ_2} \\ \hline \dfrac{B_-(z)[B_+(\zeta) - r_{p0}B_-(\zeta)]}{2iQ_1} & z. \\ \dfrac{B_-(\zeta)[B_+(z) - r_{p0}B_-(z)]}{2iQ_1} & \dfrac{B_+(z)B_-(\zeta)}{i(Q_1 + Q_2)} \end{array} \tag{29}$$

($Q_1 = q_1/\epsilon_1$ and $Q_2 = q_2/\epsilon_2$; r_{p0} is defined below.) B now satisfies an integrodifferential equation [Eq. (A.10) of Ref. 9]

$$B(z) = B_0(z) + \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v(\zeta) \left\{K^2 B(\zeta) G(z, \zeta) + \frac{\mathrm{d}B}{\mathrm{d}\zeta}\frac{\partial G}{\partial \zeta}\right\}, \tag{30}$$

where $\Delta v = 1/\epsilon - 1/\epsilon_0$ and

$$B_0(z) = \begin{cases} \exp(iq_1 z) - r_{p0}\exp(-iq_1 z) & (z < 0) \\ \sqrt{\dfrac{\epsilon_2}{\epsilon_1}}\, t_{p0}\exp(iq_2 z) & (z > 0) \end{cases}. \tag{31}$$

Here[9]

$$-r_{p0} = \frac{Q_1 - Q_2}{Q_1 + Q_2}, \qquad \sqrt{\frac{\epsilon_2}{\epsilon_1}}\, t_{p0} = \frac{2Q_1}{Q_1 + Q_2}. \tag{32}$$

An exact expression for r_p is obtained from Eq. (30) by extracting the coefficient of $\exp(-iq_1 z)$ as $z \to -\infty$. This is [cf. I (35)]

$$r_p = r_{p0} - \frac{1}{2iQ_1}\int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v \left(K^2 B B_0 + \frac{\mathrm{d}B}{\mathrm{d}\zeta}\frac{\mathrm{d}B_0}{\mathrm{d}\zeta}\right) \tag{33}$$

and may be rewritten as

$$\Delta r_p = -\frac{1}{2iQ_1}\int_{-\infty}^{\infty} \mathrm{d}\zeta\, (\Delta v K^2 B B_0 - \Delta\epsilon C C_0), \tag{34}$$

where $\Delta\epsilon = \epsilon - \epsilon_0$, $C = \mathrm{d}B/\epsilon\mathrm{d}z$, $C_0 = \mathrm{d}B_0/\epsilon_0\mathrm{d}z$. The first-order perturbation expression is obtained from Eq. (34) by replacing B by B_0 and C by C_0. (This is equivalent to lowest order in Δv to replacing $\mathrm{d}B/\mathrm{d}\zeta$ by $\mathrm{d}B_0/\mathrm{d}\zeta$ but is preferable since C is continuous at a discontinuity in ϵ, whereas $\mathrm{d}B/\mathrm{d}\zeta$ is not). Thus

$$\Delta r_p^{\text{pert}} = -\frac{1}{2iQ_1}\int_{-\infty}^{\infty} \mathrm{d}\zeta (\Delta v K^2 B_0^2 - \Delta\epsilon C_0^2). \tag{35}$$

The variational expression for r_p is obtained by operating on Eq. (30) with

$$\int_{-\infty}^{\infty} \mathrm{d}z \left[\Delta v K^2 B - \frac{\mathrm{d}}{\mathrm{d}z}\left(\Delta v \frac{\mathrm{d}B}{\mathrm{d}z}\right)\right]. \tag{36}$$

The resulting equation can again be put in the form $F = S$, where

$$F = \int_{-\infty}^{\infty} \mathrm{d}z \Delta v \left(K^2 B B_0 + \frac{\mathrm{d}B}{\mathrm{d}z}\frac{\mathrm{d}B_0}{\mathrm{d}z}\right) = -2iQ_1 \Delta r_p \tag{37}$$

is of first degree in the unknown B and

$$\begin{aligned} S = &\int_{-\infty}^{\infty} \mathrm{d}z \Delta v K^2 B \left[B - \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v \left(K^2 B G + \frac{\mathrm{d}B}{\mathrm{d}\zeta}\frac{\partial G}{\partial \zeta}\right)\right] \\ &+ \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v \frac{\mathrm{d}B}{\mathrm{d}z}\left[\frac{\mathrm{d}B}{\mathrm{d}z} - \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v \left(K^2 B \frac{\partial G}{\partial z} + \frac{\mathrm{d}B}{\mathrm{d}\zeta}\frac{\partial^2 G}{\partial z \partial \zeta}\right)\right] \end{aligned} \tag{38}$$

is of second degree in B. We again find that $\delta S = 2\delta F$, so $\delta(F^2/S) = 0$ and

$$\Delta r_p^{\text{var}} = -\frac{F^2/S}{2iQ_1}. \tag{39}$$

The simplest trial function for $B(z)$ is $B_0(z)$. This gives the values F_0 and S_0 for F and S, where

$$F_0 = \int_{-\infty}^{\infty} \mathrm{d}z (\Delta v K^2 B_0^2 - \Delta\epsilon C_0^2) = -2iQ_1 \Delta r_p^{\text{pert}}. \tag{40}$$

In the evaluation of S we must take care to include the $-\epsilon_0(z)\delta(z - \zeta)$ singularity in $\partial^2 G/\partial z\partial\zeta$. We find that

$$\begin{aligned} S = &\int_{-\infty}^{\infty} (\Delta v K^2 B^2 - \Delta\epsilon C^2) - K^4 \int_{-\infty}^{\infty} \mathrm{d}z \Delta v B \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta v B G \\ &+ 2K^2 \int_{-\infty}^{\infty} \mathrm{d}z \Delta v B \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta\epsilon C (\partial G/\epsilon_0 \partial\zeta) \\ &- \int_{-\infty}^{\infty} \mathrm{d}z \Delta\epsilon C \int_{-\infty}^{\infty} \mathrm{d}\zeta \Delta\epsilon C \frac{1}{\epsilon_0(z)\epsilon_0(\zeta)}\left(\frac{\partial^2 G}{\partial z \partial \zeta}\right)_r, \end{aligned} \tag{41}$$

where

$$\left(\frac{\partial^2 G}{\partial z \partial \zeta}\right)_r = \frac{\partial^2 G}{\partial z \partial \zeta} + \epsilon_0(z)\delta(z - \zeta) \tag{42}$$

is the regular part of $\partial^2 G/\partial z\partial\zeta$. The value of S_0 is now found by replacing B by B_0 and C by C_0 in Eq. (41), and the resulting variational estimate for the reflection amplitude has the form

$$\Delta r_p^{\text{var}} = \frac{F_0}{S_0}\Delta r_p^{\text{pert}}. \tag{43}$$

To second order in the interface thickness, Eq. (43) gives (after considerable reduction) the terms $r_{p1} + r_{p2}$ as given in Ref. 7, Eqs. (5) and (29). Thus the variational expression, Eq. (43), is correct to second order in the interface thickness. At grazing incidence, Δr_p^{var} tends to zero when $\epsilon_1 \neq \epsilon_2$, thus giving the correct r_p value.[8]

4. ADAPTATION OF THE HULTHÉN-KOHN VARIATIONAL METHOD TO REFLECTION PROBLEMS

We have seen that the adaptation of Schwinger's variational technique in scattering theory to reflection has led to s and p reflection amplitudes that are correct to second order in the interface thickness and are correct at grazing incidence. These desirable features have been obtained at the cost of some complexity, and we shall now show how the simpler Hulthén–Kohn variational method[10,11] of scattering theory may be adapted to reflection problems.

We begin with the s wave, for which the exact amplitude E satisfies Eq. (2), and consider the functional

$$\Phi[E_t] = \int_{-\infty}^{\infty} \mathrm{d}z E_t \left(\frac{\mathrm{d}^2 E_t}{\mathrm{d}z^2} + q^2 E_t\right) \tag{44}$$

of the trial function E_t, which we take to have the asymptotic forms

$$\exp(iq_1 z_1) + r_t \exp(-iq_1 z) \leftarrow E_t \rightarrow t_t \exp(iq_2 z). \tag{45}$$

We now write $E_t = E + \delta E$; because of Eq. (5) the asymptotic forms of δE are

$$\delta r \exp(-iq_1 z) \leftarrow \delta E \rightarrow \delta t \exp(iq_2 z), \tag{46}$$

where $\delta r = r_t - r$ and $\delta t = t_t - t$ (we drop the subscript s for the moment). We find that

$$\delta\Phi = \Phi[E + \delta E] - \Phi[E] = [E \mathrm{d}\delta E/\mathrm{d}z - \delta E \mathrm{d}E/\mathrm{d}z]_{-\infty}^{\infty}, \quad (47)$$

plus terms of second order in δE. {This result follows on two integrations by parts and use of the fact that, from Eq. (2), $\Phi[E] = 0$.} From Eqs. (5) and (46) we then obtain the result that $\delta\Phi = 2iq_1\delta r$, which can be written in the form of a variational principle:

$$\delta(\Phi - 2iq_1 r) = 0. \quad (48)$$

In the application of this principle, we use a trial E_t (and the corresponding r_t, t_t) to evaluate $\Phi[E_t]$; then from Eq. (48) we obtain

$$\Phi[E_t] - 2iq_1 r_t = \Phi[E] - 2iq_1 r + \text{higher-order terms in } \delta E. \quad (49)$$

The variational estimate for the reflection amplitude is thus

$$r^{\mathrm{var}} = r_t - \Phi[E_t]/2iq_1. \quad (50)$$

As an example, consider the simplest trial function $E_t = E_0$, the solution of Eq. (9). On writing $q^2 = q_0^2 + \Delta q^2$ and using Eq. (9) we see that

$$\Phi[E_0] = \int_{-\infty}^{\infty} \mathrm{d}z \Delta q^2 E_0^2, \quad (51)$$

which we recognize as the F_0 of Eq. (20). Thus the trial function E_0 leads to the first-order perturbation-theory result [Eq. (15)]

$$r_s^{\mathrm{var}} = r_{s0} - F_0/2iq_1. \quad (52)$$

There are corresponding results for the p wave: We define the functional

$$\Phi[B_t] = \int_{-\infty}^{\infty} \mathrm{d}z B_t \left\{ \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{\epsilon}\frac{\mathrm{d}B}{\mathrm{d}z}\right) + \left(\frac{\omega^2}{c^2} - \frac{K^2}{\epsilon}\right) B_t \right\} \quad (53)$$

of the trial function B_t. The variational principle now has the form

$$\delta(\Phi + 2iQ_1 r_p) = 0. \quad (54)$$

For the zeroth-order trial function B_0 [defined in Eq. (31)],

$$r_p^{\mathrm{var}} = r_{p0} + \Phi_0/2iQ_1 = r_{p0} - \frac{1}{2iQ_1}\int_{-\infty}^{\infty} \mathrm{d}z \Delta v \{K^2 B_0^2 + (\mathrm{d}B_0/\mathrm{d}z)^2\}. \quad (55)$$

This is not the same as the perturbation result [Eq. (35)]: there is agreement only to lowest order in $\Delta v = 1/\epsilon - 1/\epsilon_0$. In consequence, Eq. (55) does not give the correct result to first order in the interface thickness [Ref. 7, Eq. (5)] and does not agree with r_s^{var} at normal incidence.

The adaptation of the Hulthén–Kohn variational method to reflection problems is thus seen to give results that are inferior, for the simplest trial functions, to those obtained from adapting the Schwinger method. This is compensated for by the greater simplicity of the Hulthén–Kohn method, which makes possible the use of more-sophisticated trial functions.

5. COMPARISON OF THE PERTURBATION AND VARIATIONAL RESULTS

We begin with a comparison according to general criteria (for arbitrary interfacial profiles) and then look at the results for a particular model profile. The general criteria are that r_s and r_p should be equal at normal incidence (the s and p waves are then physically indistinguishable); that $r_s \to -1$ and $r_p \to 1$ at grazing incidence[8]; that r_s and r_p should be correct to second order in the interfacial thickness[7]; and that r_s and r_p be free of divergence for reflection between like media.[1] The status of the theories with respect to these general criteria is summarized in Table 1, for the case in which the input or trial functions for all three theories are E_0 and B_0.

We shall now see how the theories perform in the special case of a uniform layer of dielectric constant ϵ, located between z_1 and $z_2 = z_1 + \Delta z$. Only the s-wave reflectivity will be examined, as a function of interface thickness Δz and as a function of angle of incidence for fixed Δz. We need F_0 and S_0, and these depend on the positioning of the step profile $\epsilon_0(z)$. We assume for the moment only that this lies between z_1 and z_2. For this configuration we find the s-wave results

Table 1. Comparison According to General Properties of the Reflection Amplitudes[a]

Method	$r_p = r_s$ at Normal Incidence	$r_s \to -1$ at Grazing Incidence	$r_p \to 1$ at Grazing Incidence	r_s Correct to Second Order in Interface Thickness	r_p Correct to Second Order in Interface Thickness	r_s Free of Divergence When $\epsilon_1 = \epsilon_2$	r_p Free of Divergence When $\epsilon_1 = \epsilon_2$
Adaptation of Hulthén–Kohn variational method	no	yes(u)	yes(u)	yes(c)	no	no	no
First-order perturbation theory	yes	yes(u)	yes(u)	yes(c)	no	no	no
Adaptation of Schwinger variational method	yes	yes	yes	yes	yes	yes	yes

[a] The symbol (u) denotes a property valid only for unlike media ($\epsilon_1 \neq \epsilon_2$); the symbol (c) denotes the property being conditional on the positioning of the step profile so as to make $\lambda_1 = 0$.

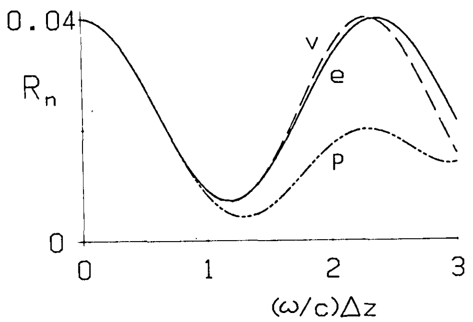

Fig. 1. Reflectivity at normal incidence, as a function of the thickness Δz of a uniform film. The exact, perturbation, and variational results are denoted by curves e, p, and v, respectively.

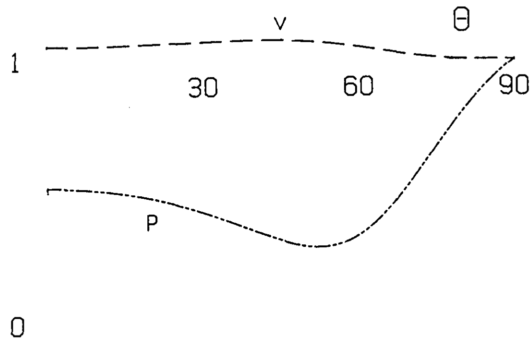

Fig. 2. Ratio of the s reflectivity estimates to the exact reflectivity, as a function of the angle of incidence. The film thickness is about one third of a wavelength ($(\omega/c)\Delta z = 2$, $\Delta z = \lambda_0/\pi$). As the reflectivity increases monotonically with angle of incidence by a factor of nearly 30, the perturbation (p) and variational (v) results show maximum deviations of about −70 and +7%.

$$F_0 = \frac{\omega^2}{c^2}\{(\epsilon-\epsilon_2)(1+r_0)^2 z_2 j_+(\phi_2) - (\epsilon-\epsilon_1)z_1[j_+(\phi_1) + 2r_0 + r_0{}^2 j_-(\phi_1)]\}, \tag{56}$$

where

$$\phi_i = q_i z_i, \qquad j_\pm(\phi) = \exp(\pm i\phi)\sin\phi/\phi; \tag{57}$$

and

$$S_0 = F_0 + 2\frac{\omega^4}{c^4}(I_{11} + I_{12} + I_{22}), \tag{58}$$

where

$$I_{11} = \left(\frac{\epsilon-\epsilon_1}{2q_1}\right)^2 z_1\{(1-r_0-r_0{}^2)[1+r_0 j_-(\phi_1)] - j_+(\phi_1) + r_0{}^3 j_-(2\phi_1) + 2r_0[r_0\exp(-2i\phi_1) - i\phi_1]\},$$

$$I_{12} = \frac{(\epsilon-\epsilon_1)(\epsilon-\epsilon_2)(1+r_0)}{(q_1+q_2)} z_1 z_2 i j_+(\phi_2)[1+r_0 j_-(\phi_1)],$$

$$I_{22} = \left\{\frac{(\epsilon-\epsilon_2)(1+r_0)}{2q_2}\right\}^2 z_2\{j_+(\phi_2) + \exp(2i\phi_2)[r_0 j_+(\phi_2) - 1] - r_0 j_+(2\phi_2)\}. \tag{59}$$

When $\epsilon_1 = \epsilon_2$, these results reduce to those obtained in Section 5 of Ref 1.

We now specify the positioning of the step profile: the first-order perturbation result [Eq. (52)] gives, to second order in the interface thickness,

$$\Delta r_s{}^{\text{pert}} = -F_0/2iq_1 = -\frac{\omega^2/c^2}{2iq_1}\left(\frac{2q_1}{q_1+q_2}\right)^2 \times [\lambda_1 + 2iq_2\lambda_2 + \ldots]. \tag{60}$$

On comparison with the exact (to this order) r_s given in Eq. (23), we see that the perturbation result is correct to second order in the interface thickness if the relative positioning of $\epsilon(z)$ and $\epsilon_0(z)$ is chosen so as to make $\lambda_1 = 0$. This is the *equal area rule* of Ref. 4:

$$\int_{-\infty}^{0} dz(\epsilon-\epsilon_1) = \int_0^\infty dz(\epsilon_2-\epsilon), \tag{61}$$

which can always be satisfied if ϵ is real and $\epsilon_1 \neq \epsilon_2$. For the profile under consideration, this condition implies that

$$z_1 = -\frac{\epsilon_2-\epsilon}{\epsilon_2-\epsilon_1}\Delta z, \qquad z_2 = \frac{\epsilon-\epsilon_1}{\epsilon_2-\epsilon_1}\Delta z. \tag{62}$$

The question of optimum positioning of the reference profile is discussed further in the next section. Here we simply compare the results obtained using the condition (61). The first-order perturbation theory and the adaptation of the Hulthén–Kohn variational theory results are equivalent for the s wave and are denoted by p in Figs. 1 and 2. The results from the adaptation of the Schwinger variational theory are denoted by v. The exact results (given in Refs. 2–4) are denoted by e. The figures illustrate the dependence of $R_s = |r_s|^2$ on interface thickness, and of $R_s/R_s{}^{\text{exact}}$ on angle of incidence, for the values $\epsilon_1 = 1$, $\epsilon = (4/3)^2$, $\epsilon_2 = (3/2)^2$, representing reflection from a layer of water on glass.

6. DISCUSSION

We see from Table 1 that the adaptation of Schwinger's variational theory to reflection problems has provided estimates for the s and p reflection amplitudes that satisfy all the currently known and verifiable general criteria. From the figures we see that the variational result is a considerable improvement on the perturbation result for the same input wave function.

We mentioned above the problem of the optimum positioning of the reference profile. For the variational methods, this positioning is an implicit variational parameter. We have not yet succeeded in solving the optimization problem in a general way, except in the long-wave limit, where the equal area rule gives the optimum positioning for the perturbation theory, whereas the adaptation of Schwinger's method is correct to second order in the interface thickness for all positionings. Our numerical experiences is that the perturbation results are sensitive to the positioning of ϵ_0 (and can be much worse than displayed in Figs. 1 and 2), whereas the variational results are insensitive to this positioning.

The theory given here clearly works best for interfaces that are thinner than a wavelength. Work is in progress on a perturbation-variation theory that can cope with thick interfaces as well.

REFERENCES

1. J. Lekner, "Reflection of light by a nonuniform film between like media," J. Opt. Soc. Am. A **3**, 9–15 (1986).
2. J. Lekner, "Reflection of long waves by interfaces," Physica **112A**, 544–556 (1982).
3. M. Born and E. Wolf, *Principles of Optics* (Pergamon, Oxford, 1965).
4. R. M. A. Azzam and N. M. Bashara, *Ellipsometry and Polarized Light* (North-Holland, Amsterdam, 1977).
5. J. Schwinger, "A variational principle for scattering problems," Phys Rev. **72**, 742 (1947).
6. J. M. Blatt and J. D. Jackson, "On the interpretation of neutron-proton scattering data by the Schwinger variational method," Phys Rev. **26**, 18–28 (1949).
7. J. Lekner, "Invariant formulation of the reflection of long waves by interfaces," Physica **128A**, 229–252 (1984).
8. J. Lekner, "Reflection at oblique incidence, and the existence of a Brewster angle," J. Opt. Soc. Am. A **2**, 186–188 (1985).
9. J. Lekner, "Second-order ellipsometric coefficients," Physica **113A**, 506–520 (1982).
10. W. Kohn, "Variational methods in nuclear collision problems," Phys Rev. **74**, 1763–1772 (1948).
11. C. J. Joachain, *Quantum Collision Theory* (North-Holland, Amsterdam, 1975).