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REFLECTION OF LONG WAVES BY INTERFACES

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We derive comparison identities for waves satisfying the equation $d^2\psi/dz^2 + q^2(z)\psi = 0$. One of these identities is used to show that to second order in the product (wavenumber component normal to interface)×(interface thickness), the reflection amplitude is given by $r = (1 - 2q_1q_2l^2)(q_1 - q_2)/(q_1 + q_2)$, where l is a length determined by the deviation of the interface profile from a step, and q_1, q_2 are the normal components of the wave numbers in media 1 and 2 on either side of the interface. For the continuous interfaces discussed, l is about two-fifths of the 10–90 interface thickness. The corresponding formula for the transmission amplitude is $t = (1 + \frac{1}{2}(q_1 - q_2)^2l^2)2q_1/(q_1 + q_2)$.

1. Introduction

The problem of interest is the reflection of waves by planar interfaces. We have in mind in particular (a) the reflection of particles of energy E by a potential $V(z)$, with the probability amplitude Ψ satisfying Schrödinger's equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi, \tag{1}$$

and (b) the reflection of electromagnetic waves (light, for example) by an interface between two media, described by a dielectric function $\epsilon(z)$. In the electromagnetic case, there are two polarizations to be considered: the s-wave, with electric field $\boldsymbol{E}$ perpendicular to the plane of incidence, and the p-wave, with the magnetic field $\boldsymbol{B}$ perpendicular to the plane of incidence. In the s-wave case, if the propagation is in the zx plane, $\boldsymbol{E} = (0, E_y, 0)$ and E_y satisfies[1])

$$\nabla^2E_y + \epsilon\frac{\omega^2}{c^2}E_y = 0, \tag{2}$$

where c is the speed of light, and ω is the angular frequency of the (monochromatic) wave. We can consider (1) and (2) together (the p-wave has special character, and will be discussed in section 5). Since V and ϵ are taken

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to be functions of z only, and Ψ and E_y are independent of y for plane waves propagating in the zx plane, both Ψ and E_y are of the form $e^{iKx}\psi(z)$, with ψ satisfying

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

where

$$q^2(z) = \begin{cases} \dfrac{2m}{\hbar^2}[E - V(z)] - K^2 & \text{(quantum particle wave)}, \\[2ex] \epsilon(z)\dfrac{\omega^2}{c^2} - K^2 & \text{(electromagnetic s-wave)}. \end{cases} \tag{4}$$

Consider a wave originating in medium 1 and incident on an interface between media 1 and 2. A reflected and a transmitted wave are set up, and in the steady state ψ has the limiting forms

$$e^{iq_1z} + r\,e^{-iq_1z} \leftarrow \psi \rightarrow t\,e^{iq_2z}, \tag{5}$$

where

$$q^2(z) = \begin{cases} \dfrac{2m}{\hbar^2}(E - V_i) - K^2, \\[2ex] \epsilon_i\dfrac{\omega^2}{c^2} - K^2. \end{cases} \tag{6}$$

The (separation of variables) constant K is the x-component of the wavevector in either medium, so if θ_1 and θ_2 are the angles of incidence and refraction, $K = k_1 \sin\theta_1 = k_2 \sin\theta_2$ (Snell's law), where

$$k_i^2 = q_i^2 + K^2 = \begin{cases} \dfrac{2m}{\hbar^2}[E - V_i], \\[2ex] \epsilon_i\dfrac{\omega^2}{c^2}. \end{cases} \tag{7}$$

Thus q_i is the component of the wavevector normal to the interface:

$$q_1 = k_1 \cos\vartheta_1 \leftarrow q(z) \rightarrow q_2 = k_2 \cos\vartheta_2. \tag{8}$$

Eq. (5) defines the reflection amplitude r and the transmission amplitude t. If the transition between the media is discontinuous, so that $q(z)$ becomes a step function, r and t are readily determined from the continuity of ψ and $d\psi/dz$ at the interface. (For example, if $d\psi/dz$ were discontinuous, $d^2\psi/dz^2$ would be a delta function, so (3) would not be satisfied). If the interface is located at $z = 0$, these conditions read $1 + r = t$ and $iq_1(1 - r) = iq_2 t$, giving the well-known results

$$r_{\text{step}} = \frac{q_1 - q_2}{q_1 + q_2}, \quad t_{\text{step}} = \frac{2q_1}{q_1 + q_2}. \tag{9}$$

When the interface thickness is small compared to the reciprocal of the wavenumber component normal to the medium, the reflection amplitude can be expected to be r_{step} plus a small correction term, dependent on the deviation of the profile from a step profile. This idea is developed here, by means of a comparison identity derived in the next section.

2. Comparison identities for reflection and transmission amplitudes

Let ψ_0 be the solution for a reference profile $q_0^2(z)$, and ψ the solution for $q^2(z)$; q_0 and q have the same values q_1 and q_2 deep inside the two media. On multiplying the wave equation for ψ_0 by ψ, and the wave equation for ψ by ψ_0, and subtracting, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\psi \frac{\mathrm{d}\psi_0}{\mathrm{d}z} - \psi_0 \frac{\mathrm{d}\psi}{\mathrm{d}z}\right) = (q^2 - q_0^2)\psi\psi_0. \tag{10}$$

Now we integrate from a point z_1 deep inside medium 1, to a point z_2 deep inside medium 2 (z_1 and z_2 are such that ψ and ψ_0 have attained their asymptotic forms of eq. (5)). The integral of the left-hand side of (10) gives $2iq_1\,(r_0 - r)$, all dependence on z_1 and z_2 cancelling out. Thus

$$r = r_0 - \frac{1}{2iq_1} \int_{-\infty}^{\infty} \mathrm{d}z(q^2 - q_0^2)\psi\psi_0, \tag{11}$$

where we have replaced z_1 and z_2 by $\mp\infty$. Similar identities have been used in discussion of two-body scattering and binding[2]).

Our results for the reflection of long waves are based on (11), but we will note in passing other identities that relate reflection and transmission amplitudes which may be derived in a similar way. Comparing the complex conjugate of ψ_0 with ψ gives

$$2iq_1(1 - rr_0^*) - 2iq_2 tt_0^* = \int_{-\infty}^{\infty} \mathrm{d}z(q^2 - q_0^2)\psi\psi_0^*. \tag{12}$$

On setting $q = q_0$, this leads to the condition known as flux conservation in quantum mechanics:

$$q_1(1-|r|^2) = q_2|t|^2. \tag{13}$$

Comparing ψ_0 with $\overleftarrow{\psi}$, a wave incident from medium 2:

$$\overleftarrow{t}\ \mathrm{e}^{-\mathrm{i}q_1 z} \leftarrow \overleftarrow{\psi} \rightarrow \mathrm{e}^{-\mathrm{i}q_2 z} + \overleftarrow{r}\ \mathrm{e}^{\mathrm{i}q_2 z} \tag{14}$$

gives

$$2\mathrm{i}(q_2 t_0 - q_1 \overleftarrow{t}) = \int_{-\infty}^{\infty} \mathrm{d}z (q^2 - q_0^2) \overleftarrow{\psi} \psi_0. \tag{15}$$

When $q_0 = q$, this gives

$$q_2 t = q_1 \overleftarrow{t}, \tag{16}$$

so (15) can be written in a form similar to (11):

$$t = t_0 - \frac{1}{2\mathrm{i}q_2} \int_{-\infty}^{\infty} \mathrm{d}z (q^2 - q_0^2) \overleftarrow{\psi} \psi_0. \tag{17}$$

Eq. (16), which relates the $1 \rightarrow 2$ and $1 \leftarrow 2$ transmission amplitudes, is implicit in the relations derived by Landau and Lifshitz[3]); it applies only to the case where q_1 and q_2 are real (for example in the case where q_2 is imaginary, the asymptotic form of $\overleftarrow{\psi}$ as given by (14) is not valid). Comparing ψ with $\overleftarrow{\psi}_0$ gives a relation like (17), with $\psi \overleftarrow{\psi}_0$ in the integrand. Finally, comparing $\overleftarrow{\psi}$ with ψ_0^* gives

$$-2\mathrm{i}(q_2 \overleftarrow{r} t_0^* + q_1 \overleftarrow{t} r_0^*) = \int_{-\infty}^{\infty} \mathrm{d}z (q^2 - q_0^2) \overleftarrow{\psi} \psi_0^*. \tag{18}$$

Setting $q = q_0$ gives $q_2 \overleftarrow{r} t^* + q_1 \overleftarrow{t} r^* = 0$, which together with (16) shows that

$$\overleftarrow{r} = -\frac{t}{t^*} r^*. \tag{19}$$

Thus the reflection amplitudes $1 \rightarrow 2$ and $1 \leftarrow 2$ have equal absolute value (again only for q_1, q_2 real)[3]).

3. Reflection amplitude for long waves

The identities derived above can be applied at any wavelength for any shape of profile. Their use in determining r and t is dependent on the availability of an exact solution ψ_0 for a profile of similar characteristics. Here we are interested in the reflection of long waves, for example the reflection of light of 5000 Å wavelength from a liquid-vapour interface which may have a thickness as small as 5 Å. In such circumstances the wave reflects, to a very good approximation, from a step interface, and the natural choice for q_0 is q_{step}. Thus we will use the identity (11) in the form

$$r = r_{\text{step}} - \frac{1}{2iq_1} \int_{-\infty}^{\infty} dz(q^2 - q_{\text{step}}^2)\psi\psi_{\text{step}}. \tag{20}$$

On Taylor-expanding $\psi\psi_{\text{step}}$ about z_{step},

$$r = r_{\text{step}} - \frac{1}{2iq_1} \int_{-\infty}^{\infty} dz(q^2 - q_{\text{step}}^2) \sum_{n=0}^{\infty} \frac{(z - z_{\text{step}})^n}{n!} \left(\frac{d^n(\psi\psi_{\text{step}})}{dz^n}\right)_{\text{step}}. \tag{21}$$

[The expansion is unorthodox, in that the second derivative of ψ_{step} is discontinuous at the step and so (for example) the third derivative has a delta-function term. But this delta-function is multiplied by $(z\text{-}z_{\text{step}})^3$ and gives zero contribution to the integral.]

Provided the step profile is located somewhere within the profile of interest, the correction to r_{step} is a power series in qa, where q is the normal component of the wavenumber in either medium, and a is a length characterizing the thickness of the interface. The $n = 0$ term in this series is proportional to $\int_{-\infty}^{\infty} dz(q^2 - q_{\text{step}}^2)$, and this can be made zero by appropriate choice of the relative positions of the profile under study and of the step profile (see fig. 1).

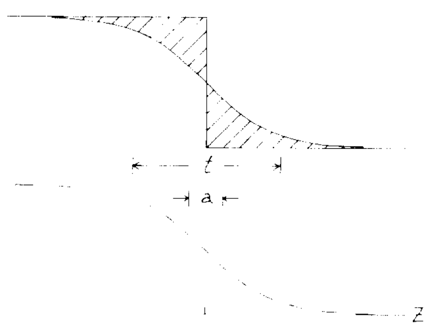


Fig. 1. Plot of $q^2(z)$ for light incident on a water–air interface. The profile shown is the Fermi function of eq. (32). Water is on the left (with $\epsilon_1 \approx (4/3)^2$), air on the right ($\epsilon_2 \approx 1$). The curve at the top is for normal incidence. A step profile is shown located so as to make the two hatched areas equal [eq. (22)]. Since $q^2 = k^2 - K^2$, the oblique incidence case is obtained by uniformly lowering the normal incidence curve. When q_2^2 becomes negative the wave incident from medium 1 is totally reflected. The lower (dashed) curve is drawn for $q_2 = 0$, i.e. at the critical angle of incidence, $\theta_1 = \arcsin(3/4)$. Also shown on the diagram are the length a of eq. (32), and the 10–90 thickness $t = (2 \log 9)\ a$.

This equal-area construction has the effect of making $\Delta r = r - r_{\text{step}}$ *second order* in qa, i.e. when

$$\int_{-\infty}^{\infty} \mathrm{d}z(q^2 - q_{\text{step}}^2) = 0. \tag{22}$$

$\Delta r = \mathcal{O}(qa)^2$. In the appendix we show (see (A.8)) that $\Delta\psi = \psi - \psi_{\text{step}}$ is of order qa, so we can replace ψ by ψ_{step} in (21) and retain r correct to second order in qa.

The origin has not yet been located. It is natural to choose it at the step, so that (from (5) and (9)) $\psi_{\text{step}}(0) = 2q_1/(q_1 + q_2)$, $(\mathrm{d}\psi_{\text{step}}/\mathrm{d}z)_0 = 2\mathrm{i}q_1q_2/(q_1 + q_2)$. Then (21) and (22) give

$$\begin{aligned} r &= r_{\text{step}} - \frac{4q_1q_2}{(q_1+q_2)^2}\int_{-\infty}^{\infty} \mathrm{d}z\, z(q^2 - q_{\text{step}}^2) + \mathcal{O}(qa)^3 \\ &= \left(\frac{q_1 - q_2}{q_1 + q_2}\right)(1 - 2q_1q_2l^2) + \mathcal{O}(qa)^3, \end{aligned} \tag{23}$$

where

$$l^2 = 2\int_{-\infty}^{\infty} \mathrm{d}z\, z(q^2 - q_{\text{step}}^2)/(q_1^2 - q_2^2) = 2\int_{-\infty}^{\infty} \mathrm{d}z\, z(k^2 - k_{\text{step}}^2)/(k_1^2 - k_2^2) \tag{24}$$

(the last equality follows from $k^2 = q^2 + K^2$). In the Schrödinger case

$$l^2 = 2\int_{-\infty}^{\infty} \mathrm{d}z\, z(V_{\text{step}} - V)/(V_2 - V_1), \quad \text{with} \int_{-\infty}^{\infty} \mathrm{d}z(V_{\text{step}} - V) = 0, \tag{25}$$

In the electromagnetic case

$$l^2 = 2\int_{-\infty}^{\infty} \mathrm{d}z\, z(\epsilon - \epsilon_{\text{step}})/(\epsilon_1 - \epsilon_2), \quad \text{with} \int_{-\infty}^{\infty} \mathrm{d}z(\epsilon - \epsilon_{\text{step}}) = 0. \tag{26}$$

Note that, by an integration by parts, with $u = V$ or ϵ,

$$l^2 = \int_{-\infty}^{\infty} \mathrm{d}z \frac{\mathrm{d}u}{\mathrm{d}z} z^2 \bigg/ \int_{-\infty}^{\infty} \mathrm{d}z \frac{\mathrm{d}u}{\mathrm{d}z} = \int_{u_1}^{u_2} \mathrm{d}u\, z^2(u) \bigg/ \int_{u_1}^{u_2} \mathrm{d}u, \tag{27}$$

so that, for a monotonic profile, l^2 is positive and for real q_i the reflection is always weaker (to second order in qa) than from a step profile. The results stated above are valid for arbitrary (not necessarily monotonic) profiles which are *non-singular*: delta function terms in $V(z)$ or $\epsilon(z)$ are excluded, for example.

The transmission amplitude t may be calculated to the same order as r from the comparison identity (17), using the step function as reference, and approximating ψ by ψ_{step}. We find, using (22), that

$$t = t_{\text{step}} + \frac{q_1 - q_2}{q_1 + q_2} \int_{-\infty}^{\infty} \mathrm{d}z\, z(q^2 - q_{\text{step}}^2) + \mathcal{O}(qa)^3$$

$$= \frac{2q_1}{q_1 + q_2}\{1 + \tfrac{1}{2}(q_1 - q_2)^2 l^2\} + \mathcal{O}(qa)^3. \tag{28}$$

Note that the flux conservation condition (13) is satisfied to the order shown. As may be expected, a profile with positive l^2 (for example, one which is monotonic) will give more transmission in the long wavelength limit than a step profile of the same height.

4. Examples

For the first two profiles the exact reflection amplitude can be expressed in terms of elementary functions:

Two-step (or uniform layer)

$$\epsilon(z) = \begin{cases} \epsilon_1, & z < -a, \\ \dfrac{a\epsilon_1 + b\epsilon_2}{a + b} \equiv \epsilon_i, & -a < z < b, \\ \epsilon_2, & z > b; \end{cases} \tag{29}$$

$$l^2 = ab = \frac{(\epsilon_1 - \epsilon_i)(\epsilon_i - \epsilon_2)}{(\epsilon_1 - \epsilon_2)^2}(a + b)^2. \tag{30}$$

The exact reflection amplitude, found by imposing the continuity of ψ and $\mathrm{d}\psi/\mathrm{d}z$ at $-a$ and b is

$$r = \mathrm{e}^{-2\mathrm{i}q_1 a}\frac{q(q_1 - q_2)\mathrm{c} + \mathrm{i}(q^2 - q_1 q_2)\mathrm{s}}{q(q_1 + q_2)\mathrm{c} - \mathrm{i}(q^2 + q_1 q_2)\mathrm{s}}, \tag{31}$$

where

$$q^2 = \frac{aq_1^2 + bq_2^2}{a + b}, \quad \begin{Bmatrix}\mathrm{c}\\ \mathrm{s}\end{Bmatrix} = \begin{matrix}\cos\\ \sin\end{matrix}\{q(a + b)\}.$$

A straightforward calculation shows that (23) and (30) agree with (31).

Fermi function (or hyperbolic tangent):

$$\epsilon(z) = \frac{\epsilon_1 + \epsilon_2\, e^{z/a}}{1 + e^{z/a}} = \frac{\epsilon_1}{1 + e^{z/a}} + \frac{\epsilon_2}{1 + e^{-z/a}}$$
$$= \tfrac{1}{2}(\epsilon_1 + \epsilon_2) - \tfrac{1}{2}(\epsilon_1 - \epsilon_2)\tanh(z/2a), \tag{32}$$

$$l^2 = \frac{\pi^2}{3} a^2. \tag{33}$$

The wave equation for this profile is soluble in terms of hypergeometric functions[3-5]), and the exact reflection amplitude is given by (with $qa = y$)

$$r = -\frac{\Gamma(2iy_1)\Gamma(-i(y_1 + y_2))\Gamma(-i(y_1 - y_2))\sinh \pi(y_1 - y_2)}{\Gamma(-2iy_1)\Gamma(i(y_1 + y_2))\Gamma(i(y_1 - y_2))\sinh \pi(y_1 + y_2)}. \tag{34}$$

Using the Weierstrass infinite product representation[6]) of the gamma function,

$$\frac{1}{\Gamma(z)} = z\, e^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right) e^{-z/n}, \tag{35}$$

where γ is Euler's constant, we find

$$\Gamma(-iy)/\Gamma(iy) = -\exp 2i\{\gamma y - \phi(y)\}, \tag{36}$$

where

$$\phi(y) = \sum_{n=1}^{\infty} \left(\frac{y}{n} - \arctan\frac{y}{n}\right). \tag{37}$$

Thus the phase of r is $2[\phi(2y_1) - \phi(y_1 + y_2) - \phi(y_1 - y_2)]$ and since $\phi(y) \sim y^3$ at small y, the phase is of the order $(qa)^3$ at long wavelengths, and (23, 33) are in agreement with (34).

In table 1 below, we compare four profiles characterized by a single length a and a function f which has the limiting values ± 1 at $\pm\infty$:

$$\epsilon(z) = \tfrac{1}{2}(\epsilon_1 + \epsilon_2) - \tfrac{1}{2}(\epsilon_1 - \epsilon_2) f(z/a) \tag{38}$$

In terms of f,

$$l^2 = \frac{a^2}{2} \int_{-\infty}^{\infty} dx\, x^2 \frac{df}{dx}. \tag{39}$$

A convenient measure of interface size is t, the 10–90 thickness[7]), defined as the distance in which $\epsilon(z)$ goes from $\epsilon_1 - (\epsilon_1 - \epsilon_2)/10$ to $\epsilon_2 + (\epsilon_1 - \epsilon_2)/10$ i.e. from $9\epsilon_1/10 + \epsilon_2/10$ to $\epsilon_1/10 + 9\epsilon_2/10$. Thus t is the difference between the z-values at which $f = \pm 4/5$. This is compared with l and a in the table:

TABLE I

Profile	$f(x)$	l/a	t/a	l/t
Linear	$\begin{cases} x & \lvert x\rvert < 1 \\ \pm 1 & \lvert x\rvert > 1 \end{cases}$	$\frac{1}{\sqrt{3}}$	$\frac{8}{5}$	0.3608
Exponential	$(1 - e^{-\lvert x\rvert})\operatorname{sgn} x$	$\sqrt{2}$	$2 \log 5$	0.4394
Fermi	$\tanh \frac{x}{2}$	$\frac{\pi}{\sqrt{3}}$	$2 \log 9$	0.4127
Error function	$\operatorname{erf}(x)$	$\frac{1}{\sqrt{2}}$	1.8124	0.3901

5. Discussion

We have derived comparison identities relating the reflection and transmission amplitudes of two arbitrary interfacial profiles. When one of these (the reference profile) is a step function, we obtain the reflection and transmission amplitudes for long waves:

$$r = \frac{q_1 - q_2}{q_1 + q_2}\{1 - 2q_1 q_2 l^2\} + \mathcal{O}(qa)^3,$$

$$t = \frac{2q_1}{q_1 + q_2}\{1 + \tfrac{1}{2}(q_1 - q_2)^2 l^2\} + \mathcal{O}(qa)^3. \tag{40}$$

When the wavelength is long compared to the thickness of the interface, a profile can therefore be characterised by a single length l, given by (with $u = V(z)$ or $\epsilon(z)$)

$$l^2 = 2\int_{-\infty}^{\infty} \mathrm{d}z\, z(u - u_{\text{step}})/(u_1 - u_2), \qquad \int_{-\infty}^{\infty} \mathrm{d}z(u - u_{\text{step}}) = 0,$$

or

$$l^2 = \int_{-\infty}^{\infty} \mathrm{d}z\, z^2 \frac{\mathrm{d}u}{\mathrm{d}z}\Big/(u_2 - u_1), \qquad \int_{-\infty}^{\infty} \mathrm{d}z\, z\frac{\mathrm{d}u}{\mathrm{d}z} = 0. \tag{41}$$

In quantum-mechanical language, the latter expression gives l^2 in terms of the second moment of the force $F(z) = -\mathrm{d}V/\mathrm{d}z$. In wave terms, the reflection is determined (to this order) by the second moment of the gradient of the square of the local wavenumber.

Our discussion (in section 1) of reflection and transmission at oblique incidence showed that q_1 and q_2 have the same role at oblique incidence as k_1 and k_2 at normal incidence. It follows that whenever (for dielectric functions of type (38)) the reflection or transmission coefficients are known for normal incidence, those for oblique incidence can be obtained by replacing k_1 by $k_1 \cos\theta_1$ and k_2 by $k_2 \cos\theta_2$.

The formulae (40) and (41) appear to be new, but they lie hidden in very old results, being implicit in the work of Maclaurin[8]) and Lord Rayleigh[9]) who obtained formal expressions for the reflection of electromagnetic waves to second order in the interface thickness. Later Abeles[10]) and Drazin[11]) rederived and extended these results, which however remained complex compared to (40) and (41). We give one example: Drazin obtains the reflection amplitude (for one-dimensional propagation) to second order in the interface thickness in terms of integrals I_1 and I_2. The first of these is proportional to (in our notation)

$$\int_{-\infty}^{\infty} dz[u(z) - u_1] + \int_{0}^{\infty} dz[u(z) - u_2],$$

which we write as $\int_{-\infty}^{\infty} dz[u - u_{\text{step}}]$. As discussed in section 3, this integral can be made zero by appropriate positioning of the step profile. Drazin's second integral I_2 is the difference between two double integrals: I_2 is proportional to

$$\int_{0}^{\infty} dz \int_{z}^{\infty} dz'[u(z') - u_2] - \int_{-\infty}^{0} dz \int_{-\infty}^{z} dz'[u(z') - u_1].$$

This reduces to $\int_{-\infty}^{\infty} dz z[u - u_{\text{step}}]$ and is thus proportional to our l^2.

We note in conclusion that the electromagnetic p-wave may be put into the form (3). For the p-wave, in the geometry of section 1, $B = (0, B_y, 0)$, $B_y = e^{iKx}B(z)$, and $B(z)$ satisfies the equation

$$\frac{d^2B}{dz^2} - \frac{1}{\epsilon}\frac{d\epsilon}{dz}\frac{dB}{dz} + \left(\epsilon\frac{\omega^2}{c^2} - K^2\right)B = 0, \tag{42}$$

which we can write in the form

$$\frac{1}{\epsilon}\frac{d}{dz}\left(\frac{1}{\epsilon}\frac{dB}{dz}\right) + \left(\frac{q}{\epsilon}\right)^2 B = 0. \tag{43}$$

Thus in terms of a new variable Z, defined by

$$dZ = \epsilon dz, \tag{44}$$

the p-wave equation becomes (with $Q = q/\epsilon$)

$$\frac{d^2B}{dZ^2} + Q^2B = 0. \tag{45}$$

There are however special problems associated with the p-wave, which will be discussed elsewhere[12]).

Appendix

Perturbation theory for reflection problems

We wish to express ψ, the solution of

$$\frac{d^2\psi}{dz^2} + q^2\psi = 0, \quad e^{iq_1 z} + r e^{-iq_1 z} \leftarrow \psi \rightarrow t\, e^{iq_2 z} \tag{A.1}$$

in terms of a known function ψ_0, the solution of

$$\frac{d^2\psi_0}{dz^2} + q_0^2\psi_0, \quad e^{iq_1 z} + r_0 e^{-iq_1 z} \leftarrow \psi_0 \rightarrow t_0\, e^{iq_2 z}. \tag{A.2}$$

Write $q^2 = q_0^2 + \Delta q^2$, and $\psi = \psi_0 + \psi_1 + \psi_2 + \dots$ (a series of powers of Δq^2). From (A.1) and (A.2), ψ_1 satisfies the equation

$$\frac{d^2\psi_1}{dz^2} + q_0^2\psi_1 = -\Delta q^2\psi_0. \tag{A.3}$$

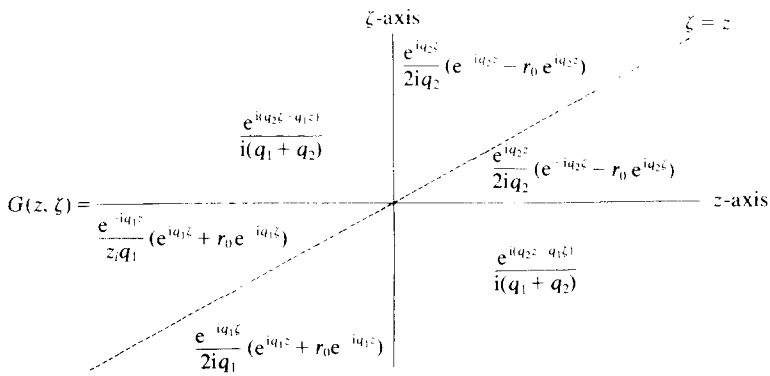
To solve (A.3) we need to construct a Green's function $G(z, \zeta)$ satisfying

$$\frac{\partial^2 G}{\partial z^2} + q_0^2(z)G = \delta(z - \zeta). \tag{A.4}$$

Then

$$\psi_1(z) = -\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta)\psi_0(\zeta)G(z, \zeta). \tag{A.5}$$

For long waves, the physical choice for q_0 is q_{step}, and the Green's function satisfying (A.4) and incorporating the required boundary conditions is (with $r_0 = (q_1 - q_2)/(q_1 + q_2)$)



(A.6)

From (A.5) and (A.6), we find the asymptotic form of $\psi_1(z)$ as $z \to -\infty$:

$$\psi_1(z) \to e^{-iq_1 z}\left\{\frac{i}{2q_1}\int_{-\infty}^{0} d\zeta \Delta q^2(\zeta)(e^{iq_1\zeta} + r_0\, e^{-iq_1\zeta})^2 + \frac{i}{q_1+q_2}\int_{0}^{\infty} d\zeta \Delta q^2(\zeta) \times (e^{iq_1\zeta} + r_0 e^{-iq_1\zeta}) e^{iq_2\zeta}\right\}. \quad \text{(A.7)}$$

Comparison with (A.1) then gives the first-order (in Δq^2) correction to the reflection amplitude. Writing $r = r_0 + r_1 + r_2 + \ldots$, we identify r_1 as the expression inside the braces in (A.7). In the long-wave limit,

$$r_1 = \frac{2iq_1}{(q_1+q_2)^2}\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta) - \frac{\Delta q_1 q_2}{(q_1+q_2)^2}\int_{-\infty}^{\infty} d\zeta\, \zeta \Delta q^2(\xi) + \mathcal{O}(qa)^3. \quad \text{(A.8)}$$

The first term is in agreement with the $n = 1$ term of (21) when ψ is approximated by ψ_{step}. The next term is in agreement with (23) only when (22) is satisfied ($\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta) = 0$): in general $r - r_{\text{step}}$ contains a term second order in Δq^2 in the $\mathcal{O}(qa)^2$ expression. To see this, we look at higher order perturbations. The nth order (in Δq^2) correction ψ_n satisfies the equation

$$\frac{d^2\psi_n}{dz^2} + q_0^2\psi_n = -\Delta q^2 \psi_{n-1}, \quad \text{(A.9)}$$

which is of the same form as (A.3). Thus ψ_2 is given by (A.5) with ψ_1 replacing ψ_0. The asymptotic form as $z \to -\infty$ is

$$\psi_2(z) \to e^{-iq_1 z}\left\{\frac{i}{2q_1}\int_{-\infty}^{0} d\zeta \Delta q^2(\zeta)\psi_1(\zeta)(e^{iq_1\zeta} + r_0 e^{-iq_1\zeta}) + \frac{i}{q_1+q_2}\int_{0}^{\infty} d\zeta \Delta q^2(\zeta)\psi_1(\zeta)\, e^{iq_2\zeta}\right\}. \quad \text{(A.10)}$$

The expression inside the braces is r_2. In the long-wave limit,

$$r_2 \to \frac{i\psi_1(0)}{q_1+q_2}\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta) \quad \text{(A.11)}$$

and from (A.5) and (A.6),

$$\psi_1(0) \to \frac{2iq_1}{(q_1+q_2)^2}\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta). \quad \text{(A.12)}$$

Thus

$$r_2 \to \frac{-2q_1}{(q_1+q_2)^3}\left(\int_{-\infty}^{\infty} d\zeta \Delta q^2(\zeta)\right)^2, \tag{A.13}$$

which demonstrates that the reflection amplitude to $\mathcal{O}(qa)^2$ contains (in general) a term second order in Δq^2. The simplicity of the result (23) is thus seen to follow from the positioning of the step profile to make $\int_{-\infty}^{\infty} d\zeta \Delta q^2 = 0$.

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References

1) L.D. Landau and E.M. Liftshitz, Electrodynamics of Continuous Media (Pergamon, Oxford, 1960), §68.
2) J. Lekner, Mol. Phys. **23** (1972) 619.
3) L.D. Landau and E.M. Lifshitz, Quantum Mechanics (Pergamon, Oxford, 1965), §25.
4) C. Eckart, Phys. Rev. **35** (1930) 1303.
5) P.S. Epstein, Proc. Natl. Acad. Sci. **16** (1930) 627.
6) E.T. Whittaker and G.N. Watson, A Course of Modern Analysis (Cambridge, 1963), §12.1.
7) J. Lekner and J.R. Henderson, Physica **94A** (1978) 545.
8) R.C. Maclaurin, Proc. Roy. Soc. **A76** (1905) 49.
9) Lord Rayleigh, Proc. Roy. Soc. **A86** (1912) 207.
10) F. Abelès, Annales de Physique **5** (1950) 596.
11) P.G. Drazin, Proc. Roy. Soc. **A273** (1963) 400.
12) J. Lekner, Physica A, to be published.