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# Variational Theory of Reflection

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*Abstract*

Schwinger's variational method for the scattering phase shift produced by a central potential is adapted to reflection by a planar potential barrier (or well). The formulation is general, for an arbitrary transition between any two media, but the application here is limited to reflection at a barrier between media of equal potential energy. The simplest variational estimate for the reflection amplitude correctly tends to $-1$ at grazing incidence, as it must for any finite barrier. This is in contrast to the first order perturbation reflection amplitude, which diverges at grazing incidence. The same variational estimate is also correct to second order in the ratio of the interface thickness to the wavelength of the incident wave. The theory applies also to the reflection of the electromagnetic s (or transverse electric) wave at an interface between two media.

## 1. Introduction

The variational theory developed here gives an estimate of (for example) the reflection amplitude of electron waves at an oxide barrier between two metals or of electromagnetic s waves at an interface between two dielectrics. The formulation is general, but the application will be limited to an important special case: the reflection at a barrier or interface between like media. Two examples of this special case are: the reflection of electrons at an oxide barrier between the *same* metal, and reflection of light by a soap film in air.

The quantum and electrodynamic problems described above are mathematically identical, since in each case one is dealing with a linear second order partial differential equation of the same form. For particles of mass $m$ and energy $E$ moving in a potential $V(z)$, the probability amplitude satisfies Schrödinger's equation

$$-(\hbar^2/2m)\nabla^2\Psi+V\Psi = E\Psi\,. \tag{1}$$

For electromagnetic s (or transverse electric) waves propagating in the $xz$ plane and moving in a medium with dielectric function $\varepsilon(z)$, the electric field is $(0, E_y, 0)$, and $E_y$ satisfies

$$\nabla^2 E_y+\varepsilon(\omega^2/c^2)E_y = 0\,, \tag{2}$$

where $c$ is the speed of light and $\omega$ is the angular frequency of the monochromatic wave (see e.g. Landau and Liftshitz 1960, Sect. 68).

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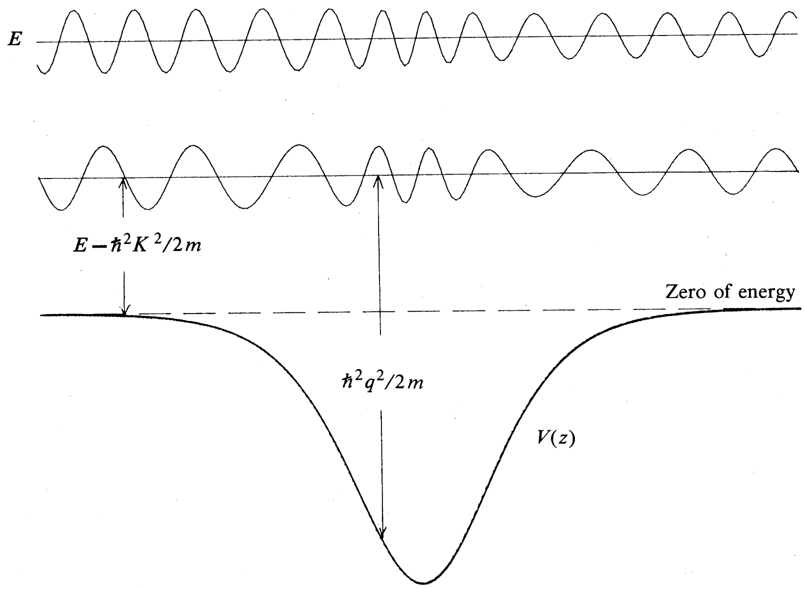


**Fig. 1.** Reflection of a particle of mass $m$ at a planar potential inhomogeneity. The potential energy function (lower curve) is $V = \Delta V \operatorname{sech}^2(z/a)$, as discussed in Section 5. The upper curve is a schematic representation of the $z$ variation of the wavefunction for normal incidence; the middle curve is for incidence at 45°.

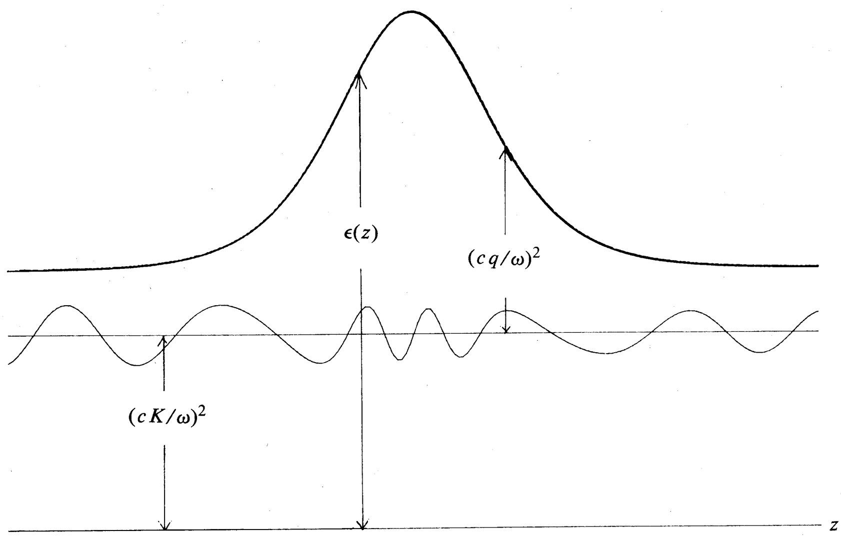


**Fig. 2.** Reflection of an electromagnetic wave of angular frequency $\omega$ at a planar inhomogeneity in the dielectric function $\varepsilon$ (upper curve). The lower curve is a schematic representation of the wavefunction at an angle of incidence of 60°. The dielectric function is given by $\varepsilon = 1+\operatorname{sech}^2(z/a)$; reflection for this type of profile is discussed in Section 5.

Since $V$ and $\varepsilon$ are taken to be functions of $z$ only, and $\Psi$ and $E_y$ are independent of $y$ for plane waves propagating in the $xz$ plane, both $\Psi$ and $E_y$ are of the form $\exp(\mathrm{i}Kx)\,\psi(z)$, with $\psi$ satisfying

$$d^2\psi/dz^2 + q^2\psi = 0, \tag{3}$$

where

$$q^2(z) = (2m/\hbar^2)\{E - V(z)\} - K^2 \quad \text{(quantum particle wave)} \tag{4a}$$

$$q^2(z) = \varepsilon(z)(\omega^2/c^2) - K^2 \quad \text{(electromagnetic s wave)}. \tag{4b}$$

The separation of variables constant $K$ is $k_\parallel$, the $x$ component of the wave vector in either medium, so if $\theta_1$ and $\theta_2$ are the angles of incidence and refraction, then $K = k_1 \sin\theta_1 = k_2 \sin\theta_2$ (Snell's law), where for $i = 1, 2$

$$k_i^2 = q_i^2 + K^2 = (2m/\hbar^2)(E - V_i) \quad \text{(quantum particle wave)} \tag{5a}$$

$$k_i^2 = q_i^2 + K^2 = \varepsilon_i \omega^2/c^2. \quad \text{(electromagnetic s wave)}. \tag{5b}$$

Thus $(1 - V_i/E)^{\frac{1}{2}}$ or $\varepsilon_i^{\frac{1}{2}}$ are the refractive indices for the two media. The component of the wave vector normal to the interface is $q(z)$, with limiting forms

$$q_1 = k_1 \cos\theta_1 \leftarrow q(z) \rightarrow k_2 \cos\theta_2 = q_2. \tag{6}$$

The reflection of particles at a planar potential well, and of electromagnetic waves at a planar inhomogeneity in the dielectric function, are illustrated in Figs 1 and 2.

The reflection amplitude $r$ and the transmission amplitude $t$ are defined in terms of the asymptotic forms of the solution of (3):

$$\exp(\mathrm{i}q_1 z) + r\exp(-\mathrm{i}q_1 z) \leftarrow \psi \rightarrow t\exp(\mathrm{i}q_2 z), \tag{7}$$

and satisfy the flux conservation law (provided $q_1$ and $q_2$ are real)

$$q_1(1 - |r|^2) = q_2 |t|^2 \tag{8}$$

(see e.g. Landau and Lifshitz 1965, Sect. 25).

We shall derive and apply a variational principle for $r$. Since the proof uses the Green function approach of perturbation theory, and since it will be instructive to compare the perturbation and variational approaches, we shall first give a brief review of the former.

## 2. Perturbation Theory for Reflection Problems

We wish to express $\psi$, the solution of (3) and (7), in terms of a known function $\psi_0$, the solution of

$$d^2\psi_0/dz^2 + q_0^2\psi_0 = 0, \tag{9a}$$

$$\exp(\mathrm{i}q_1 z) + r_0 \exp(-\mathrm{i}q_1 z) \leftarrow \psi_0 \rightarrow t_0 \exp(\mathrm{i}q_2 z). \tag{9b}$$

This is done in terms of a Green function $G(z, \zeta)$ satisfying

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

We then have

$$\psi(z) = \psi_0(z) - \int_{-\infty}^{\infty} d\zeta\, \Delta q^2(\zeta)\, G(z,\zeta)\, \psi(\zeta), \tag{11}$$

where $\Delta q^2 = q^2 - q_0^2$. We now iterate (11) so that successive iterations give successive orders (in $\Delta q^2$) in the expansion $\psi = \psi_0 + \psi_1 + \psi_2 + \ldots$. To first order in $\Delta q^2$ we obtain

$$\psi_1(z) = -\int_{-\infty}^{\infty} d\zeta\, \Delta q^2(\zeta)\, G(z,\zeta)\, \psi_0(\zeta). \tag{12}$$

The choice of $q_0(z)$ (and thus of $\psi_0$ and $G$) depends on the problem. In the simplest case of like media on either side of the interface, the natural choice is $q_0$ constant, equal to the common value of $q_1$ and $q_2$. Then, we have

$$r_0 = 0, \quad \psi_0(z) = \exp(i q_0 z), \quad G(z,\zeta) = (1/2i q_0)\exp(i q_0 |z-\zeta|). \tag{13}$$

This case was discussed by Morse and Feshbach (1953, p. 1071). The first order perturbation value for the reflection amplitude is obtained from (12) by taking the limit $z \to -\infty$ and extracting the coefficient of $\exp(-i q_0 z)$:

$$r_1 = -\frac{1}{2i q_0} \int_{-\infty}^{\infty} d\zeta\, \Delta q^2(\zeta) \exp(2i q_0 \zeta). \tag{14}$$

We note that $r_1$ diverges as $q_0 \to 0$ (at grazing incidence).

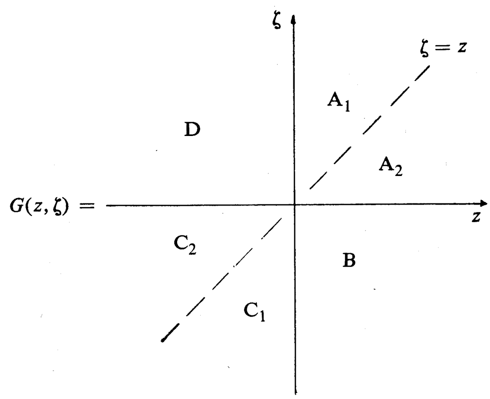


**Fig. 3.** Six analytic parts of the Green function in the $z\zeta$ plane:
A$_1$: $(2i q_2)^{-1} \exp(i q_2 \zeta)\{\exp(-i q_2 z) - r_0 \exp(i q_2 z)\}$
A$_2$: $(2i q_2)^{-1} \exp(i q_2 z)\{\exp(-i q_2 \zeta) - r_0 \exp(i q_2 \zeta)\}$
B: $\{i(q_1 + q_2)\}^{-1} \exp\{i(q_2 z - q_1 \zeta)\}$
C$_1$: $(2i q_1)^{-1} \exp(-i q_1 \zeta)\{\exp(i q_1 z) + r_0 \exp(-i q_1 z)\}$
C$_2$: $(2i q_1)^{-1} \exp(-i q_1 z)\{\exp(i q_1 \zeta) + r_0 \exp(-i q_1 \zeta)\}$
D: $\{i(q_1 + q_2)\}^{-1} \exp\{i(q_2 \zeta - q_1 z)\}$.

The general case of unlike media ($q_1 \neq q_2$) has recently been studied by Lekner (1982*a*). For long waves, the natural choice for $q_0(z)$ is the step function ($q_0 = q_1$ for $z < 0$ and $q_0 = q_2$ for $z > 0$), for which

$$\psi_0(z) = \exp(i q_0 z) + r_0 \exp(-i q_0 z), \quad z < 0 \tag{15a}$$

$$\psi_0(z) = t_0 \exp(\mathrm{i}\, q_0 z), \qquad z > 0, \tag{15b}$$

where

$$r_0 = (q_1 - q_2)/(q_1 + q_2), \qquad t_0 = 2q_1/(q_1 + q_2). \tag{16, 17}$$

For this problem the Green function has six analytic parts, as shown in Fig. 3. The reflection amplitude is $r = r_0 + r_1 + \dots$, where the first order part $r_1$ is found from (12) and Fig. 3 to be*

$$r_1 = \frac{\mathrm{i}}{2q_1} \int_{-\infty}^{0} \mathrm{d}\zeta\, \Delta q^2(\zeta) \{\exp(\mathrm{i}\, q_1 \zeta) + r_0 \exp(-\mathrm{i}\, q_1 \zeta)\}^2$$
$$+ \frac{\mathrm{i}}{q_1 + q_2} \int_{0}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, t_0 \exp(2\mathrm{i}\, q_2 \zeta). \tag{18}$$

Higher order parts of the reflection amplitude may be obtained from the limiting form of

$$\psi_n(z) = -\int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, G(z, \zeta)\, \psi_{n-1}(\zeta), \tag{19}$$

but they rapidly become complicated.

## 3. Variational Estimate for the Reflection Amplitude

In this section we adapt Schwinger's variational method for the tangent of the phase shift produced by scattering off a central potential (Schwinger 1947; Blatt and Jackson 1949). As in the perturbation theory, $\psi$ is taken to be the solution of (3) and (7), $\psi_0$ the solution of (9), and $G$ the solution of (10). We rewrite (11) as

$$\psi(z) + \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, G(z, \zeta)\, \psi(\zeta) = \psi_0(z). \tag{20}$$

On multiplication by $\Delta q^2(z)\,\psi(z)$ and integration over the whole range of $z$, we obtain

$$\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi^2(z) + \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi(z) \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, \psi(\zeta)\, G(z, \zeta)$$
$$= \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi(z)\, \psi_0(z). \tag{21}$$

We write this as $\mathsf{S} = \mathsf{F}$, where $\mathsf{S}$ (the left side of 21) is of second degree in $\psi$, and $\mathsf{F}$ (the right side of 21) is of first degree in $\psi$. Now $\psi$ satisfies the integral equation (11); the asymptotic form of $\psi$ as $z \to -\infty$ is found from (11) and Fig. 3 to be

$$\exp(\mathrm{i}\, q_1 z) + \exp(-\mathrm{i}\, q_1 z)\left(r_0 - \frac{1}{2\mathrm{i}\, q_1} \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, \psi(\zeta)\, \psi_0(\zeta)\right)$$
$$\equiv \exp(\mathrm{i}\, q_1 z) + r \exp(-\mathrm{i}\, q_1 z). \tag{22}$$

* A misprint in the second term in (A7) of Lekner (1982*a*) has been corrected in equation (18).

It follows that, for the exact $\psi$,

$$\mathsf{F} = 2\mathrm{i}\, q_1 (r_0 - r)\,. \tag{23}$$

For the exact $\psi$, we also have $\mathsf{S} = \mathsf{F}$. We consider now a shift to a neighbouring function (in the variational sense) $\psi + \delta\psi$, where $\psi$ is the exact solution. The integrals $\mathsf{F}$ and $\mathsf{S}$ shift by

$$\delta \mathsf{F} = \int_{-\infty}^{\infty} \mathrm{d}z\, \delta\psi(z)\, \Delta q^2(z)\, \psi_0(z)\,, \tag{24}$$

$$\begin{aligned} \delta \mathsf{S} &= 2\int_{-\infty}^{\infty} \mathrm{d}z\, \delta\psi(z)\, \Delta q^2(z) \left( \psi(z) + \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, G(z,\zeta)\, \psi(\zeta) \right) \\ &= 2\int_{-\infty}^{\infty} \mathrm{d}z\, \delta\psi(z)\, \Delta q^2(z)\, \psi_0(z)\,. \end{aligned} \tag{25}$$

Thus $\delta\mathsf{S} = 2\delta\mathsf{F}$. But because $\mathsf{S} = \mathsf{F}$, so $\delta\mathsf{S}/\mathsf{S} = 2\delta\mathsf{F}/\mathsf{F}$, or

$$\delta(\mathsf{F}^2/\mathsf{S}) = 0\,. \tag{26}$$

This is the variational principle: the correct $\psi$ will extremize $\mathsf{F}^2/\mathsf{S}$. The extremal value of $\mathsf{F}^2/\mathsf{S}$ approximates $\mathsf{F} = 2\mathrm{i}\, q_1(r_0 - r)$ and thus we have a variational value for the reflection amplitude:

$$r^{\mathrm{var}} = r_0 - \mathsf{F}^2/2\mathrm{i}\, q_1\, \mathsf{S}\,. \tag{27}$$

In general one has a parametrized trial function $\psi^{\mathrm{var}}(z)$, which when substituted for $\psi(z)$ gives the values $\mathsf{F}^{\mathrm{var}}$ and $\mathsf{S}^{\mathrm{var}}$; the parameters which extremize $(\mathsf{F}^{\mathrm{var}})^2/\mathsf{S}^{\mathrm{var}}$ then give the best value (in the space spanned by the trial function) of the reflection amplitude. However, a useful variational estimate can be obtained without any parameters in $\psi^{\mathrm{var}}$, provided $\psi^{\mathrm{var}}$ is well chosen. For example, we can take $\psi^{\mathrm{var}} = \psi_0$. This gives a value for $r^{\mathrm{var}}$ which corresponds (in terms of the input or trial function) to the first-order perturbation value $r$:

$$r_1^{\mathrm{var}} = -\left(\frac{F_0^2}{2\mathrm{i}\, q_1}\right) \Big/ \left( F_0 + \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi_0(z) \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, \psi_0(\zeta)\, G(z,\zeta) \right), \tag{28}$$

where (from equation 18)

$$\begin{aligned} F_0 &= \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi_0^2(z) \\ &= \int_{-\infty}^{0} \mathrm{d}z\, \Delta q^2(z) \{\exp(\mathrm{i}\, q_1 z) + r_0 \exp(-\mathrm{i}\, q_1 z)\}^2 \\ &\quad + \left(\frac{2q_1}{q_1 + q_2}\right)^2 \int_0^{\infty} \mathrm{d}z\, \Delta q^2(z) \exp(2\mathrm{i}\, q_2 z) \\ &= -2\mathrm{i}\, q_1 r_1\,. \end{aligned} \tag{29}$$

Thus, we have

$$r_1^{\mathrm{var}} = r_1 \Big/ \left( 1 + \frac{\mathrm{i}}{2q_1 r_1} \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\, \psi_0(z) \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\, \psi_0(\zeta)\, G(z,\zeta) \right). \tag{30}$$

The numerator $r_1$ is first order in $\Delta q^2$, as is the second term in the denominator, and thus $r_1$ and $r_1^{\text{var}}$ agree to first order. A special situation arises when $r_1$ is divergent; one example of this will be discussed in the next section.

## 4. Reflection at an Interface between Like Media

Here we set $q_0$ equal to the common value of $q_1$ and $q_2$, $r_0$ equal to zero, and let $\psi_0(z) = \exp(\mathrm{i}q_0 z)$ and $G(z,\zeta) = \exp(\mathrm{i}q_0|z-\zeta|)/2\mathrm{i}q_0$. Then $r_1$ is given by (14), and (30) simplifies to

$$r_1^{\text{var}} = r_1 \Big/ \left(1 + \frac{1}{4q_0^2 r_1}\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\exp(\mathrm{i}q_0 z) \times \int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\exp(\mathrm{i}q_0\zeta)\exp(\mathrm{i}q_0|z-\zeta|)\right). \tag{31}$$

At grazing incidence ($q_0 \to 0$), $r_1$ diverges. This is unphysical: $r$ must stay within the unit circle in the complex plane. But $r_1^{\text{var}}$ does not diverge and, in fact, $r^{\text{var}} \to -1$ at grazing incidence, the correct limiting value for any finite reflecting potential. [This result follows from the general expression for the reflection amplitude (Lekner 1982*b*, equation 18) on setting $q_1 = 0$.]

The variational expression for $r$ based on the trial function has another desirable property: it is exact to second order in the interface thickness. The reflection amplitude to second order in the interface thickness is known for an arbitrary interface profile (Lekner 1984). When $q_1 = q_2$ the general expression reduces to

$$r = \frac{\mathrm{i}}{2q_0}\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z) - \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z) z + \left(\frac{\mathrm{i}}{2q_0}\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\right)^2 + \dots, \tag{32}$$

where the series continues to higher order terms in the interface thickness. From (14) we have

$$r_1 = \frac{\mathrm{i}}{2q_0}\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z) - \int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z) z + \dots. \tag{33}$$

Also, we have

$$\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\exp(\mathrm{i}q_0 z)\int_{-\infty}^{\infty} \mathrm{d}\zeta\, \Delta q^2(\zeta)\exp(\mathrm{i}q_0\zeta)\exp(\mathrm{i}q_0|z-\zeta|) = \left(\int_{-\infty}^{\infty} \mathrm{d}z\, \Delta q^2(z)\right)^2 + \dots. \tag{34}$$

On substituting equations (33) and (34) into (31) we regain (32).

Since $r_1^{\text{var}}$ is the same as $r_1$ to first order in $\Delta q^2$, and is correct to second order in the interface thickness, we expect this variational estimate to work best for weak reflection, and for interfaces whose thickness is small compared with the wavelength. In fact, the practical range of validity of (31) can be greater than this, as shown by the example in the next section.

## 5. Application to the $\mathrm{sech}^2(z/a)$ Potential

The wave equation for motion of a particle in the potential

$$V(z) = V_0 + \Delta V \,\mathrm{sech}^2(z/a) \tag{35}$$

is solvable in terms of the hypergeometric function (Landau and Lifshitz 1965, pp. 79, 80). For motion in one dimension, with particle energy $E = V_0 + \hbar^2 k_0^2/2m$, the reflection amplitude is given by

$$r = \frac{\Gamma(\mathrm{i}k_0 a)\Gamma(-s-\mathrm{i}k_0 a)\Gamma(1+s-\mathrm{i}k_0 a)}{\Gamma(-\mathrm{i}k_0 a)\Gamma(1+s)\Gamma(-s)}, \tag{36}$$

where

$$s = \tfrac{1}{2}\{-1+(1-8ma^2\Delta V/\hbar^2)^{\frac{1}{2}}\}. \tag{37}$$

The above applies to reflection at normal incidence. From (3) and (4) we see that for reflection at oblique incidence the effective wave number is given by

$$q^2(z) = (2m/\hbar^2)\{E-V(z)\}-K^2,$$

with the limiting value

$$q_0^2 = (2m/\hbar^2)(E-V_0)-K^2 = k_0^2-K^2. \tag{38}$$

The differential equation for the probability amplitude, and its boundary conditions, are thus of the same form at oblique incidence as for normal incidence, with $k_0$ replaced by $q_0$. It follows that at oblique incidence the reflection amplitude is given by (36), with $k_0$ replaced by $q_0$.

We may consider at the same time the reflection of electromagnetic s waves, with the dielectric function given by

$$\varepsilon(z) = \varepsilon_0 + \Delta\varepsilon \,\mathrm{sech}^2(z/a). \tag{39}$$

The reflection amplitude is given by (36) with $q_0$ replacing $k_0$, and

$$s = \tfrac{1}{2}[-1+\{1+4\Delta\varepsilon(\omega^2/c^2)a^2\}^{\frac{1}{2}}]. \tag{40}$$

In both cases the problem is characterized by two dimensionless parameters; firstly, a coupling parameter (cf. Lekner 1972)

$$\alpha = -2ma^2\Delta V/\hbar^2 \quad \text{or} \quad \alpha = \Delta\varepsilon(\omega^2/c^2)a^2, \tag{41}$$

which is a measure of the strength and size of the reflecting inhomogeneity, and secondly, $\beta = q_0 a$, the product of the normal component of the wave number with the thickness of the barrier.

We will restrict ourselves here to real s ($\alpha \geqslant -\frac{1}{4}$) which implies $\Delta V \leqslant \hbar^2/8ma^2$ and $\Delta\varepsilon \geqslant -c^2/4\omega^2a^2$ (there is no restriction on negative values of $\Delta V$ or positive values of $\Delta\varepsilon$). Then, using $\Gamma(z)\Gamma(1-z) = \pi/\sin\pi z$, we find

$$\begin{aligned} |r|^2 &= |\cosh\pi\beta + \mathrm{i}\cot\pi s \sinh\pi\beta|^{-2} \\ &= \frac{\cos^2\{\frac{1}{2}\pi(1+4\alpha)^{\frac{1}{2}}\}}{\cos^2\{\frac{1}{2}\pi(1+4\alpha)^{\frac{1}{2}}\}+\sinh^2\pi\beta}. \end{aligned} \tag{42}$$

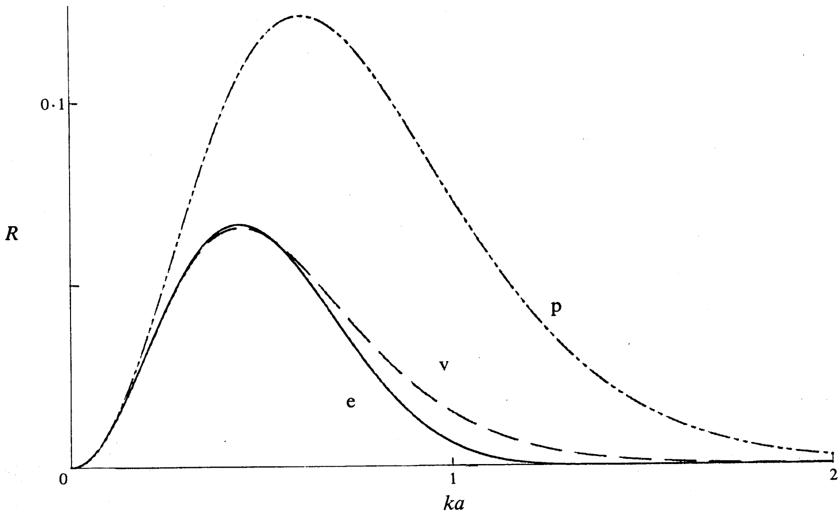


**Fig. 4.** Reflection at normal incidence at a $\mathrm{sech}^2(z/a)$ profile, for particles ($V_0 = 0, \Delta V = -E$) or electromagnetic waves ($\varepsilon_0 = 1, \Delta\varepsilon = 1$), as a function of the profile thickness. The wave number $k$ is equal to $(2mE)^{\frac{1}{2}}/\hbar$ and $\omega/c$ respectively. The solid curve gives the exact reflectivity (e) (equation 42), the dashed curve the variational estimate (v) (equation 44), and the dot–dash curve the perturbation theory expression (p) (equation 43).

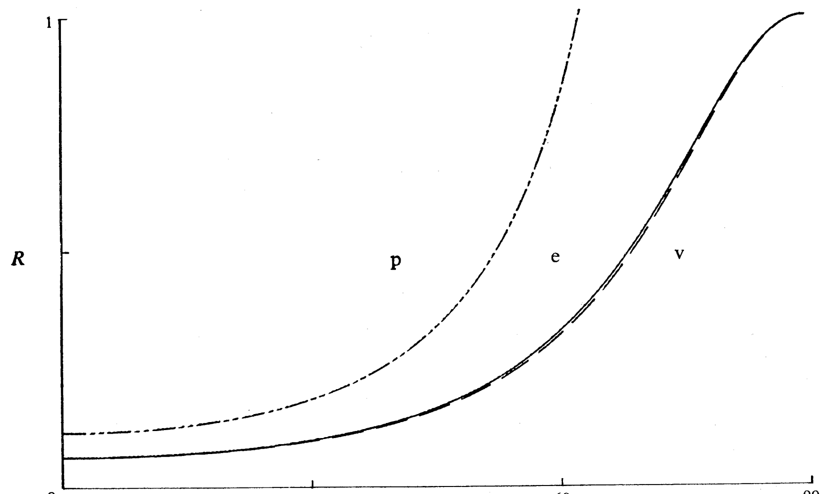


**Fig. 5.** Reflectivity as a function of the angle of incidence for the $\mathrm{sech}^2(z/a)$ profile. The exact, variational and perturbation results are denoted by e, v and p. The curves are for $\Delta V = -E$ or $\Delta\varepsilon = \varepsilon_0$, with $ka = \frac{1}{2}$ ($k$ being defined in Fig. 4). The distance over which the profiles differ by more than 10% of $|\Delta V|$ or $|\Delta\varepsilon|$ from $V_0$ or $\varepsilon_0$ is $2a\log(\sqrt{10}+3)$; for $ka = \frac{1}{2}$, this is about 0·29 times the wavelength.

The corresponding perturbation and variational expressions are (from equations 14 and 31)

$$|r_1|^2 = (\pi\alpha/\sinh\pi\beta)^2\,, \tag{43}$$

$$|r_1^{\mathrm{var}}|^2 = |r_1|^2/\{(1+\alpha)^2+(\alpha/\beta)^2\}\,. \tag{44}$$

These expressions for the reflectivity are compared in Figs 4 and 5. We note again the divergence of the perturbation theory at grazing incidence, where the variational theory gives the correct value of unit reflectivity.

## 6. Discussion

We have seen that the adaptation of Schwinger's variational method for the scattering phase shift to reflection problems gives a useful expression for the reflection amplitude, even in the simplest case of a trial function with no variational parameters. It is easy to write down more realistic trial wavefunctions. In equations (45) below, $r$ and $t$ are variational parameters, and the vertical line separates two analytic parts of the trial function. These analytic parts are to be joined at some $z_0$, which may be chosen by symmetry, e.g. $z_0 = 0$ for the example in Section 5, or which may itself be a variational parameter:

$$\exp(\mathrm{i}\,q_0\,z)\,, \tag{45a}$$

$$\exp(\mathrm{i}\,q_0\,z)+r\exp(-\mathrm{i}\,q_0\,z)\mid t\exp(\mathrm{i}\,q_0\,z)\,, \tag{45b}$$

$$\exp\{\mathrm{i}\,\phi(z)\}\,,\quad \phi(z) = \int_0^z \mathrm{d}\zeta\, q(z)\,, \tag{45c}$$

$$\exp\{\mathrm{i}\,\phi(z)\}+r\exp\{-\mathrm{i}\,\phi(z)\}\mid t\exp\{\mathrm{i}\,\phi(z)\}\,, \tag{45d}$$

$$q^{-\frac{1}{2}}(z)\exp\{\mathrm{i}\,\phi(z)\}\,, \tag{45e}$$

$$q^{-\frac{1}{2}}(z)\exp\{\mathrm{i}\,\phi(z)\}+rq^{-\frac{1}{2}}(z)\exp\{-\mathrm{i}\,\phi(z)\}\mid tq^{-\frac{1}{2}}(z)\exp\{\mathrm{i}\,\phi(z)\}\,. \tag{45f}$$

The results given here are based on (45a); even this trial function (which does not have reflection built in) leads to a variational expression for the reflection amplitude which is exact at grazing incidence, and correct to second order in the interface thickness.

The results given here are restricted to quantum particle waves and to the electromagnetic s wave. We hope in the future to also extend the theory to the electromagnetic p wave, in order to make available formulae for the interpretation of ellipsometric data on interfaces (Beaglehole 1983).

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