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# VECTOR THEORY OF LIGHT SCATTERING FROM A ROUGH SURFACE: UNITARY AND RECIPROCAL EXPANSIONS

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We present a vector theory of light scattering from a rough surface which is based on the Rayleigh solution to the electromagnetic boundary value problem. The extinction theorem is used in order to obtain the "reduced" Rayleigh equations, which involve only the field outside the medium. These equations may be written in a way that makes the unitarity and reciprocity of the theory readily apparent, and also provides a means of generating approximate solutions that satisfy this requirement. As a result, this formalism provides a convenient starting point for making flux-conserving approximations when treating the scattering of light from a randomly rough surface.

## 1. Introduction

The effect of macroscopic surface roughness on the interaction of electromagnetic waves with surfaces is believed to play a crucial role in many phenomena. For example, the coupling of p-polarized light with surface polaritons on a metal grating is known to have a dramatic effect on the optical reflectivity, and the enhancement of the surface fields is probably important in the giant Raman effect of molecules adsorbed on rough metal surfaces [1,2].

In many instances, the scale of the surface roughness is small compared to the wavelength of the incident radiation, and a perturbative solution to the problem is appropriate. There have been many such approaches developed [3], most of which have reduced the electromagnetic boundary value problem to a scalar one. Those theories which have taken into account the vector nature of the field [4] are not easily generalizable to include higher orders in the surface corrugation. It is our purpose here to present a treatment for the vector field that formally includes all orders, and is also conceptually and computationally easy to handle.

One method of solving the surface boundary value problem that has been utilized in many different areas is based on the Rayleigh ansatz. This leads to an integral equation for the field coefficients which can be expanded in powers of $p\zeta(\boldsymbol{R})$, where $\zeta(\boldsymbol{R})$ is the surface corrugation function and $p$ is the component of the wave vector perpendicular to the surface. Recent investigations into the relation between the Rayleigh method and other formulations [3,5] have shown that the conditions of convergence and practical utility of this series are separate questions from those determining the validity of the Rayleigh ansatz; hence the method provides the easiest way of obtaining an expansion of the exact solution. For radiation in the visible spectrum, we expect the method to prove useful for surface roughness on the order of 100 Å.

We will examine here the problem of light scattering from a semi-infinite medium bounded by a rough surface. Since the theory will allow for two independent polarizations of the field and a two-dimensional surface corrugation function, we will be able to treat the cross polarized scattering that has been observed in light scattering from a rough surface [6,7] in a consistent manner. An additional feature of the theory is that it includes naturally the effects of excitation and reradiation of surface polaritons.

In section 2 of this paper we derive the Rayleigh equations for a vector field. The extinction theorem is then used to eliminate the field inside the medium, and we obtain two coupled integral equations for the two independent polarizations of the diffracted amplitude. We will then, in section 3, rewrite the equations in a form that corresponds closely to the $K$ matrix formalism of scattering theory. This will enable us to find approximate solutions for the scattering amplitude which satisfy the requirements of unitarity and reciprocity.

In a separate work we will apply the theory to the scattering of light from a randomly rough surface. It is especially important that we have a unitary theory in this case, because it is the starting point for making "conserving approximations" that correctly treat the energy transport into and out of the surface polariton resonances.

## 2. The vector Rayleigh equations

In this section we formally solve the boundary value problem of an electromagnetic wave incident on a corrugated dielectric half-space. The treatment is general, incorporating the full vector nature of the electromagnetic field and a two-dimensional surface corrugation. The basic idea, following along the lines of ref. [3], is to use the Rayleigh hypothesis along with the extinction theorem to derive the "reduced" Rayleigh equations for the diffracted amplitudes.

We assume that the medium is adequately characterized by a local, frequency-dependent, complex dielectric constant $\epsilon(\omega)$. Above the corrugated surface, the relevant solution of Maxwell's equations consists of an incident wave plus the outgoing scattered waves, all having frequency $\omega$:

$$A(R,z)=\sum_K A(K)\,e^{iK\cdot R}\,e^{ipz}+A^i(K_0)\,e^{iK_0\cdot R}\,e^{-ip_0z}, \tag{2.1}$$

for $z>\zeta_{max}$ with $K^2+p^2=(\omega/c)^2$. $A$ stands for either the electric or the magnetic field, and $(K_0, -p_0)$ is the momentum of the incident wave $A^i$. Here we take the substrate to lie generally below the plane $z=0$ with the exact position of the corrugated surface given by the corrugation function $\zeta(R)$, with $R=(x,y)$. Within the dielectric $(z<\zeta_{min})$ the solution consists of a sum of plane waves traveling away from the surface;

$$C(R,z)=\sum_K C(K)\,e^{iK\cdot R}\,e^{-iqz}, \tag{2.2}$$

with $q^2+K^2=\epsilon(\omega/c)^2$.

The electric and magnetic fields must satisfy the usual boundary conditions at $z=\zeta(R)$:

$$\hat{n}\times(E^<-E^>)=0, \tag{2.3a}$$

$$\hat{n}\cdot(\epsilon^<E^<-\epsilon^>E^>)=0, \tag{2.3b}$$

$$\hat{n}\times(B^<-B^>)=0, \tag{2.4a}$$

$$\hat{n}\cdot(B^<-B^>)=0, \tag{2.4b}$$

where $\hat{n}$ is a unit vector normal to the surface (see appendix A). We assume that it is possible to solve the problem by using the Rayleigh hypothesis for both the reflected fields (2.1) and the transmitted fields (2.2), and requiring that these fields satisfy the boundary conditions (2.3) and (2.4). This procedure generates a system of equations coupling the fields outside the medium, $A$, with the fields inside, $C$. One is then faced with the difficulty of uncoupling these equations in order to obtain an equation involving only the scattered amplitudes, $A$. Therefore, we will take a different approach and use the extinction theorem in order to eliminate the fields inside the medium from the analysis.

We begin by writing down the vector Kirchhoff integral relation [8] for the fields inside and outside a dielectric medium:

$$\frac{1}{4\pi}\int_s\left[i\frac{\omega}{c}G_\epsilon(\hat{n}\times B)+(\hat{n}\times E)\times\nabla'G_\epsilon+(\hat{n}\cdot E)\nabla'G_\epsilon\right]ds'$$

$$=\begin{cases}E(r), & z<\zeta(R),\\ 0, & z>\zeta(R),\end{cases} \tag{2.5a}$$

$$E^{\mathrm{i}}(r)+\frac{1}{4\pi}\int_{S}\left[\mathrm{i}\frac{\omega}{c}G_0(\hat{n}\times B)+(\hat{n}\times E)\times\nabla' G_0+(\hat{n}\cdot E)\nabla' G_0\right]\mathrm{d}s'$$
$$=\begin{cases}E(r), & z>\zeta(R),\\ 0, & z<\zeta(R).\end{cases} \tag{2.5b}$$

The unit vector $\hat{n}$ is normal to the surface $S$; it is directed into the medium in (2.5a), and away from the medium in (2.5b). The gradient operator $\nabla'$ acts on the primed coordinates. The Green functions appearing in these equations satisfy the differential equations

$$\left[\nabla'^2+(\omega/c)^2\right]G_0(r,r')=-4\pi\delta(r-r'), \tag{2.6a}$$
$$\left[\nabla'^2+\epsilon(\omega/c)^2\right]G_\epsilon(r,r')=-4\pi\delta(r-r'), \tag{2.6b}$$

with radiative boundary conditions.

Eqs. (2.5) follow after substituting the Green functions (2.6) into Green's theorem for a vector field; eq. (2.5b) for $z<\zeta$ is referred to as the extinction theorem because it implies that sources (induced currents) are set up on the boundary surface so as to extinguish the incident field, $E^{\mathrm{i}}$, in the dielectric region, and establish a transmitted wave having a new phase velocity $v=c/\sqrt{\epsilon}$. These sources also account for the scattered fields in the vacuum region.

Using the boundary conditions (2.3) and (2.4) in eq. (2.5a), along with the fact $B=-\mathrm{i}(c/\omega)\nabla'\times E$, we can get the following relation involving only the electric field above the surface:

$$\int\left[G_\epsilon\hat{n}\times(\nabla'\times E^{>})+(\hat{n}\times E^{>})\times\nabla' G_\epsilon+\left(\hat{n}\cdot\frac{E^{>}}{\epsilon}\right)\nabla' G_\epsilon\right]\mathrm{d}s'=0,\quad z>\zeta(R). \tag{2.7}$$

The Green function $G_\epsilon(r,r')$ satisfying eq. (2.6b) with radiative boundary conditions is

$$G_\epsilon(r,r')=\frac{\mathrm{e}^{\mathrm{i}k_\epsilon|r-r'|}}{|r-r'|}, \tag{2.8a}$$

with $k_\epsilon^2=\epsilon(\omega/c)^2$. When a surface is present, it is most useful to express $G_\epsilon$ in terms of its Fourier transform in the $K$ direction (parallel to the surface):

$$G_\epsilon(r,r')=\frac{2\pi\mathrm{i}}{L^2}\sum_{K}\frac{\mathrm{e}^{\mathrm{i}q|z-z'|}}{q}\mathrm{e}^{\mathrm{i}K\cdot(R-R')}, \tag{2.8b}$$

where $K^2+q^2=\epsilon(\omega/c)^2$ and $L^2$ is the area of the surface. If $z>z'$, we can drop the absolute value; then the gradient of $G_\epsilon$ becomes

$$\nabla' G_\epsilon=-\frac{2\pi\mathrm{i}}{L^2}\sum_{K}\mathrm{i}k_\epsilon\frac{\mathrm{e}^{\mathrm{i}q(z-z')}}{q}\mathrm{e}^{\mathrm{i}K\cdot(R-R')}, \tag{2.9}$$

for $z>z'$ with $k_\epsilon=(K,q)$.

According to the Rayleigh hypothesis, we can express the electric field just above the surface as

$$E^{>}(R',z') = \sum_{K'} E^{>}(k')\, e^{iK'\cdot R'}\, e^{ip'z'}, \tag{2.10}$$

where $K'^2 + p'^2 = (\omega/c)^2$. It is convenient to include in the sum the incident field, with $K' = K_0$ and $p' = -p_0$ ($p_0 > 0$), as well as the reflected fields, with $p'$ positive real (scattered waves) or positive imaginary (evanescent waves). In either case, substituting the expressions (2.8), (2.9) and (2.10) into (2.7) with the observation point at $z = z_0 > z'$ gives

$$\sum_{K,K'} e^{iK\cdot R}\, e^{iqz_0} \int e^{-i(K-K')\cdot R} \frac{e^{i(p'-q)\zeta(R')}}{q} \times \left[ \hat{n} \times [k' \times E^{>}(k')] - [\hat{n} \times E^{>}(k')] \times k_\epsilon - \left(\hat{n} \cdot \frac{E^{>}(k')}{\epsilon}\right) k_\epsilon \right] ds' = 0. \tag{2.11}$$

After some manipulations (see appendix A), the vector products reduce to

$$\frac{i(\epsilon - 1)}{p' - q} \left[ \left(\frac{\omega}{c}\right)^2 E^{>}(k') - \frac{k_\epsilon}{\epsilon} [k_\epsilon \cdot E^{>}(k')] \right] \equiv \beta(k_\epsilon, k'), \tag{2.12}$$

and (2.11) may be rewritten as

$$\sum_{K} e^{iK\cdot R}\, e^{iqz_0} \sum_{K'} \frac{(e^{i(p'-q)\zeta})_{K-K'}}{q} \beta(k_\epsilon, k') = 0. \tag{2.13}$$

The subscript on the exponential term indicates the $K - K'$ Fourier transform.

Because this equation holds for all $R$, each term in the sum over $K$ must vanish separately:

$$\sum_{K'} \frac{(e^{i(p'-q)\zeta})_{K-K'}}{q} \beta(k_\epsilon, k') \equiv E^{<}(k_\epsilon) = 0. \tag{2.14}$$

For a given value of $K$, this factor represents the amplitude of a refracted wave $E^{<}(k_\epsilon) e^{iK\cdot R} e^{iqz_0}$ which vanishes since $z_0 > \zeta_{max}$. The amplitude $E^{<}(k_\epsilon)$ has two independent transverse polarizations which can be expressed in terms of the orthonormal vectors

$$\hat{a}_{\parallel}(k_\epsilon) = \frac{c}{\omega\sqrt{\epsilon}}(q\hat{K} - K\hat{z}), \quad \hat{a}_{\perp}(k_\epsilon) = \hat{z} \times \hat{K}, \tag{2.15}$$

so that

$$\hat{a}_{\parallel}(k_\epsilon) \cdot k_\epsilon = 0 \quad \text{and} \quad \hat{a}_{\perp}(k_\epsilon) \cdot k_\epsilon = 0.$$

Taking the dot product of the vector equation (2.14) with $\hat{a}_{\|}(\boldsymbol{k}_{\epsilon})$ and $\hat{a}_{\perp}(\boldsymbol{k}_{\epsilon})$ gives the two component equations [9]

$$\sum_{K'} \frac{(\mathrm{e}^{-\mathrm{i}(q-p')\zeta})_{K-K'}}{q-p'}\Big(\big(KK' + \hat{K}\cdot\hat{K}'p'q\big)\,A_{\|}(K') - (\hat{K}\times\hat{K}')q\frac{\omega}{c}A_{\perp}(K')\Big)$$

$$= -\frac{(\mathrm{e}^{-\mathrm{i}(q+p_0)\zeta})_{K-K_0}}{q+p_0}\Big(\big[KK_0 - (\hat{K}\cdot\hat{K}_0)p_0q\big]\,A^{\mathrm{i}}_{\|}(K_0)$$

$$-(\hat{K}\times\hat{K}_0)q\frac{\omega}{c}A^{\mathrm{i}}_{\perp}(K_0)\Big), \tag{2.16a}$$

$$\sum_{K'} \frac{(\mathrm{e}^{-\mathrm{i}(q-p')\zeta})_{K-K'}}{q-p'}\Big(1-(\hat{K}\times\hat{K}')p'\frac{\omega}{c}\,A_{\|}(K') + (\hat{K}\cdot\hat{K}')\frac{\omega^2}{c^2}\,A_{\perp}(I')\Big)$$

$$= -\frac{(\mathrm{e}^{-\mathrm{i}(q+p_0)\zeta})_{K-K_0}}{q+p_0}\Big((\hat{K}\times\hat{K}_0)p_0\frac{\omega}{c}A^{\mathrm{i}}_{\|}(K_0) + (\hat{K}\cdot\hat{K}_0)\frac{\omega^2}{c^2}\,A^{\mathrm{i}}_{\perp}(K_0)\Big). \tag{2.16b}$$

Here we have expressed the vector $E^{>}(k')$ in terms of two independent transverse polarizations as

$$E^{>}(k') = A_{\|}(K')\,\hat{a}_{\|}(k') + A_{\perp}(K')\,\hat{a}_{\perp}(k'), \tag{2.17}$$

where

$$\hat{a}_{\|}(k') = \frac{c}{\omega}(p'\hat{K}' - K'\hat{z}), \quad \hat{a}_{\perp}(k') = \hat{z}\times\hat{K}', \tag{2.18}$$

so that $\hat{a}_{\|}(k')\cdot k' = 0$ and $\hat{a}_{\perp}(k')\cdot k' = 0$ where $k' = K' + p'\hat{z}$. Also, the term associated with the incident field, $A^{\mathrm{i}}$, has been extracted from the sum.

Eqs. (2.16a) and (2.16b) are the Rayleigh equations for the vector field. The parallel polarized scattering amplitude, $A_{\|}(K')$ and the perpendicular polarized scattering amplitude, $A_{\perp}(K')$, are coupled to each other through these equations. This coupling allows the incident field to change its polarization upon scattering, and in addition will allow both types of incident field to couple to surface polaritons.

We can express the component equations (2.156a) and (2.16b) in a more compact form by using matrix notation,

$$\sum_{K',\beta} M_{\alpha\beta}(K,K')\,A_{\beta}(K') = -\sum_{\beta} N_{\alpha\beta}(K,K_0)\,A_{\beta}(K_0). \tag{2.19}$$

In the above, we have introduced a polarization index $\beta$, which takes on the values $\beta = 1$ (p-polarization) and $\beta = 2$ (s-polarization). The matrices $M(K,K')$

and $N(\boldsymbol{K},\boldsymbol{K}_0)$ are

$$M(\boldsymbol{K},\boldsymbol{K}') = \frac{\left(\mathrm{e}^{-\mathrm{i}(q-p')\zeta(\boldsymbol{R})}\right)_{\boldsymbol{K}-\boldsymbol{K}'}}{q-p'} \begin{pmatrix} KK' + (\hat{K}\cdot\hat{K}')p'q & -\frac{\omega}{c}q(\hat{K}\times\hat{K}') \\ \frac{\omega}{c}(\hat{K}\times\hat{K}')p' & \left(\frac{\omega}{c}\right)^2(\hat{K}\cdot\hat{K}') \end{pmatrix},$$

$$N(\boldsymbol{K},\boldsymbol{K}_0) = \frac{\left(\mathrm{e}^{-\mathrm{i}(q+p_0)\zeta(\boldsymbol{R})}\right)_{\boldsymbol{K}-\boldsymbol{K}_0}}{q+p_0} \begin{pmatrix} KK_0 - (\hat{K}\cdot\hat{K}_0)p_0q & -\frac{\omega}{c}q(\hat{K}\times\hat{K}_0) \\ -\frac{\omega}{c}(\hat{K}\times\hat{K}_0)p_0 & \left(\frac{\omega}{c}\right)^2(\hat{K}\cdot\hat{K}_0) \end{pmatrix}.$$

## 3. Unitary and reciprocal formulation

We will now show that (2.16) may be rearranged into a form that closely resembles conventional scattering theory. For this purpose, it will be convenient to rewrite (2.19) as

$$\sum_{\boldsymbol{K}'} M(\boldsymbol{K},\boldsymbol{K}')\mathscr{A}(\boldsymbol{K}',\boldsymbol{K}_0) = -N(\boldsymbol{K},\boldsymbol{K}_0). \tag{3.1}$$

The $2\times 2$ matrix $\mathscr{A}(\boldsymbol{K},\boldsymbol{K}_0)$ is defined as

$$\mathscr{A}(\boldsymbol{K},\boldsymbol{K}_0)_{\alpha\beta} = A(\boldsymbol{K})_\alpha / A^0(\boldsymbol{K}_0)_\beta, \tag{3.2a}$$

and the $S$-matrix elements are written in terms of this quantity as

$$S(\boldsymbol{K},\boldsymbol{K}_0)_{\alpha\beta} = (p/p_0)^{1/2}\mathscr{A}(\boldsymbol{K},\boldsymbol{K}_0)_{\alpha\beta}. \tag{3.2b}$$

Following ref. [10] we make the ansatz

$$\mathscr{A}(\boldsymbol{K},\boldsymbol{K}_0) = R(K)\,\delta(K,K_0) + 2\mathrm{i}\,f(K)\,T(\boldsymbol{K},\boldsymbol{K}_0)\,f(K_0)\,p_0, \tag{3.3a}$$

$$T(\boldsymbol{K},\boldsymbol{K}_0) = V(\boldsymbol{K},\boldsymbol{K}_0) + \sum_{\boldsymbol{K}'} T(\boldsymbol{K},\boldsymbol{K}')\,G(K')\,V(\boldsymbol{K}',\boldsymbol{K}_0). \tag{3.3b}$$

The quantities $R(K)$, $f(K)$, $G(K)$, $V(\boldsymbol{K},\boldsymbol{K}_0)$ and $T(\boldsymbol{K},\boldsymbol{K}_0)$ are understood to be $2\times 2$ matrices. $R(K)$ is simply the reflection coefficient for a smooth surface. Eqs. (3.3) and (3.1) establish a form for $V(\boldsymbol{K},\boldsymbol{K}_0)$ once $f(K)$ and $G(K)$ have been specified. We will choose these matrices to be such that the matrix $V(\boldsymbol{K},\boldsymbol{K}_0)$ is reciprocal and hermitian (for $\epsilon$ real and negative):

$$R(K) = \begin{pmatrix} \frac{\epsilon p - q}{\epsilon p + q} & 0 \\ 0 & \frac{p-q}{p+q} \end{pmatrix}, \tag{3.4a}$$

$$f(K)=\begin{pmatrix} \dfrac{\epsilon}{\epsilon p+q} & 0 \\ 0 & \dfrac{1}{p+q} \end{pmatrix}, \tag{3.4b}$$

$$G(K)=\mathrm{i}f(K). \tag{3.4c}$$

If we multiply (3.3a) from the left by $M(\boldsymbol{K}_1,\boldsymbol{K})$ and sum over $\boldsymbol{K}$, we find, using (3.1), that

$$\sum_{\boldsymbol{K}'} M(\boldsymbol{K},\boldsymbol{K}')\,f(K')\;T(\boldsymbol{K}',\boldsymbol{K}_0)$$
$$= -\left[M(\boldsymbol{K},\boldsymbol{K}_0)\;R(K_0)+N(\boldsymbol{K},\boldsymbol{K}_0)\right]\left[2\mathrm{i}f(K_0)\,p_0\right]^{-1}. \tag{3.5}$$

We then multiply (3.3b) from the left by $M(\boldsymbol{K}_1,\boldsymbol{K})f(K)$ and sum over $\boldsymbol{K}$. Using (3.5), we find

$$\left[N(\boldsymbol{K},\boldsymbol{K}_0)\,f^{-1}(K_0)+M(\boldsymbol{K},\boldsymbol{K}_0)\;R(K_0)\,f^{-1}(K_0)\right]$$
$$=2\mathrm{i}\,p_0\sum_{\boldsymbol{K}'}\left(\left[N(\boldsymbol{K},\boldsymbol{K}')\,f^{-1}(K')+M(\boldsymbol{K},\boldsymbol{K}')\;R(K')\,f^{-1}(K')\right]\frac{G(K')}{2\mathrm{i}\,p'}\right.$$
$$\left.-M(\boldsymbol{K},\boldsymbol{K}')\,f(K')\right)V(\boldsymbol{K}',\boldsymbol{K}_0). \tag{3.6}$$

Upon defining

$$h_N(K)=f^{-1}(K), \tag{3.7a}$$

$$h_M(K)=\begin{pmatrix} \dfrac{\epsilon p-q}{\epsilon} & 0 \\ 0 & p-q \end{pmatrix}, \tag{3.7b}$$

(3.6) takes the final form

$$\left[N(\boldsymbol{K},\boldsymbol{K}_0)\;h_N(K_0)+M(\boldsymbol{K},\boldsymbol{K}_0)\;h_M(K_0)\right]/2\mathrm{i}\,p_0$$
$$=\sum_{\boldsymbol{K}'}\left[N(\boldsymbol{K},\boldsymbol{K}')-M(\boldsymbol{K},\boldsymbol{K}')\right]\left(\frac{1}{2p'}\right)\;V(\boldsymbol{K}',\boldsymbol{K}_0). \tag{3.8}$$

We will now show that the $S$-matrix elements defined by (3.2) satisfy the following reciprocity condition:

$$\begin{pmatrix} S_{11}(\boldsymbol{K},\boldsymbol{K}_0) & S_{12}(\boldsymbol{K},\boldsymbol{K}_0) \\ S_{21}(\boldsymbol{K},\boldsymbol{K}_0) & S_{22}(\boldsymbol{K},\boldsymbol{K}_0) \end{pmatrix}=\begin{pmatrix} S_{11}(-\boldsymbol{K}_0,-\boldsymbol{K}) & -S_{21}(-\boldsymbol{K}_0,-\boldsymbol{K}) \\ -S_{12}(-\boldsymbol{K}_0,-\boldsymbol{K}) & S_{22}(-\boldsymbol{K}_0,-\boldsymbol{K}) \end{pmatrix}. \tag{3.9}$$

The appearance of the negative signs on the off diagonal elements of the reciprocal matrix is due to the fact that when the direction of the propagation vector $\boldsymbol{k}=\boldsymbol{K}+p\hat{z}$ is reversed, the s-polariztion vector $\hat{z}\times\hat{K}$ also changes sign, whereas the p-polarization vector $(c/\omega)(p\hat{K}-K\hat{z})$ does not.

In what follows, for a matrix $A$ we define its reciprocal $\tilde{A}$ by the operation (3.9); that is, $\boldsymbol{K} \to -\boldsymbol{K}_0$, $\boldsymbol{K}_0 \to -\boldsymbol{K}$, and the off diagonal elements are interchanged and multiplied by $-1$. We also have $\widetilde{(AB)} = \tilde{B}\tilde{A}$.

From the definition of the $S$-matrix (3.2b), it can be seen that $S = \tilde{S}$ if $V = \tilde{V}$. Since eq. (3.8) is of the form $IV = D$, $V = \tilde{V}$ if $I\tilde{D} = D\tilde{I}$ [10]. This implies that the following condition on $M$ and $N$ must be satisfied:

$$\sum_{\boldsymbol{K}'}\left[M(\boldsymbol{K},\boldsymbol{K}')\frac{1}{p'}\tilde{N}(\boldsymbol{K}',\boldsymbol{K}_0) - N(\boldsymbol{K},\boldsymbol{K}')\frac{1}{p'}\tilde{M}(\boldsymbol{K}',\boldsymbol{K}_0)\right] = 0. \tag{3.10}$$

Eq. (3.10) represents three conditions; two of these involve the diagonal elements and the third involves the off-diagonal elements. Written out explicitly they are

$$\begin{aligned}\sum_{\boldsymbol{K}'}\frac{1}{p'}\Big(&F^{+}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')\Big\{\big[KK' + (\hat{K}\cdot\hat{K}')p'q\big]\big[K'K_0 - (\hat{K}'\cdot\hat{K}_0)p'q_0\big]\\ &+ (\hat{K}\times\hat{K}')\cdot(\hat{K}'\times\hat{K}_0)qq_0\left(\frac{\omega}{c}\right)^2\Big\}\\ &- F^{-}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')\Big\{\big[KK' - (\hat{K}\cdot\hat{K}')p'q\big]\big[K'K_0 + (\hat{K}'\cdot\hat{K}_0)p'q_0\big]\\ &+ (\hat{K}\times\hat{K}')\cdot(\hat{K}'\times\hat{K}_0)qq_0\left(\frac{\omega}{c}\right)^2\Big\}\Big) = 0,\end{aligned} \tag{3.11a}$$

$$\begin{aligned}\sum_{\boldsymbol{K}'}\frac{1}{p'}&\big[F^{+}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}') - F^{-}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')\big]\Big[(\hat{K}\times\hat{K}')\cdot(\hat{K}'\times\hat{K}_0)p'^2\\ &- (\hat{K}\cdot\hat{K}')(\hat{K}'\cdot\hat{K}_0)\left(\frac{\omega}{c}\right)^2\Big] = 0,\end{aligned} \tag{3.11b}$$

$$\begin{aligned}\sum_{\boldsymbol{K}'}\frac{1}{p'}\Big(&F^{+}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')\Big\{\big[KK' + (\hat{K}\cdot\hat{K}')p'q\big](\hat{K}'\times\hat{K}_0)_z p'\\ &+ (\hat{K}\times\hat{K}')_z(\hat{K}'\cdot\hat{K}_0)q\left(\frac{\omega}{c}\right)^2\Big\}\\ &+ F^{-}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')\Big\{\big[KK' - (\hat{K}\cdot K')p'q\big](\hat{K}'\times\hat{K}_0)_z p'\\ &- (\hat{K}\times\hat{K}')_z(\hat{K}'\cdot\hat{K}_0)q\left(\frac{\omega}{c}\right)^2\Big\}\Big) = 0,\end{aligned} \tag{3.11c}$$

where

$$F^{+}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}') = \frac{(\mathrm{e}^{-\mathrm{i}(q-p')\zeta(\boldsymbol{R})})_{\boldsymbol{K}-\boldsymbol{K}'}}{q-p'}\,\frac{(\mathrm{e}^{-\mathrm{i}(q_0+p')\zeta(\boldsymbol{R})})_{\boldsymbol{K}'-\boldsymbol{K}_0}}{q_0+p'}. \tag{3.11d}$$

$F^{-}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')$ is obtained from $F^{+}(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')$ by letting $p' \to -p'$. To show that the conditions (3.11) are true, we follow the method of ref. [10] which will only briefly outline here. First, we write out the Fourier transforms explicitly in (3.11d) and introduce a vector $\boldsymbol{\alpha}$ so that

$$F^+(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}') = \frac{1}{(q-p')(q_0+p')}\int \mathrm{d}^2R_1\,\mathrm{d}^2R_2\,\mathrm{e}^{\mathrm{i}(\boldsymbol{K}_0\cdot\boldsymbol{R}_2-\boldsymbol{K}\cdot\boldsymbol{R}_1)}$$
$$\times\,\mathrm{e}^{\mathrm{i}\boldsymbol{K}'\cdot(\boldsymbol{R}_1-\boldsymbol{R}_2+\boldsymbol{\alpha})}\,\mathrm{e}^{-\mathrm{i}[q\zeta(\boldsymbol{R}_1)+q_0\zeta(\boldsymbol{R}_2)]}\,\mathrm{e}^{\mathrm{i}p'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]}\Big|_{\boldsymbol{\alpha}=0}. \tag{3.12}$$

Upon performing certain manipulations on (3.11), and using $p'^2=(\omega/c)^2-K'^2$, we will find that all powers of $\boldsymbol{K}'$ can be written as derivatives with respect to $\boldsymbol{\alpha}$; the sum over $\boldsymbol{K}'$ can then be performed, giving us expressions like

$$(\nabla_\alpha)^m\int \mathrm{d}^2R_1\,f(\boldsymbol{R}_1,\boldsymbol{\alpha})\,[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_1+\boldsymbol{\alpha})]^n, \tag{3.13}$$

to be evaluated at $\boldsymbol{\alpha}=0$. As long as $m<n$, what remains is a power series in $\boldsymbol{\alpha}$ with no constant terms; hence, the desired result follows. The method is sound provided that the sum over $\boldsymbol{K}'$ converges, and if the order of summation and integration can be interchanged. We have shown [10] that this can be done if the Rayleigh series converges. The manipulations required to obtain expressions like (3.13) from (3.11) are somewhat lengthy, and are outlined in appendix B. Eqs. (3.11) are indeed satisfied, so that the effective potential, and hence $T(\boldsymbol{K},\boldsymbol{K}')$, are self-reciprocal.

If $\epsilon$ is real and negative, no energy can be transported into the medium. Hence, the $S$-matrix must be unitary:

$$\sum_{\boldsymbol{K}'} S^*(\boldsymbol{K}',\boldsymbol{K})\,S(\boldsymbol{K}',\boldsymbol{K}_0)=\delta(\boldsymbol{K},\boldsymbol{K}_0). \tag{3.14}$$

The sum over $\boldsymbol{K}'$ is, of course, restricted to open channels ($K'^2<(\omega/c)^2$). We note that since $f(K)=f^*(K)R(K)$ (open channels) we may write

$$S(\boldsymbol{K},\boldsymbol{K}_0)=S'(\boldsymbol{K},\boldsymbol{K}_0)\,R(K_0), \tag{3.15a}$$

$$S'(\boldsymbol{K},\boldsymbol{K}_0)=\delta(\boldsymbol{K},\boldsymbol{K}_0)+2\mathrm{i}\sqrt{pp_0}\,f(K)\,T(\boldsymbol{K},\boldsymbol{K}_0)\,f^*(K_0), \tag{3.15b}$$

so that (3.14), using $R(K_0)R^*(K_0)=1$, becomes equivalent to

$$\sum_{\boldsymbol{K}'} S'^*(\boldsymbol{K}',\boldsymbol{K})\,S'(\boldsymbol{K}',\boldsymbol{K}_0)=\delta(\boldsymbol{K},\boldsymbol{K}_0). \tag{3.16}$$

As in conventional scattering theory, (3.16) follows from the optical theorem for $T(\boldsymbol{K},\boldsymbol{K}_0)$, which in turn is valid if the effective potential $V(\boldsymbol{K},\boldsymbol{K}')$ is hermitian. Details are given in appendix C.

To show that $V=V^\dagger$, we first note the following:

$$M^\dagger(\boldsymbol{K},\boldsymbol{K}')=\begin{cases}-\tilde{N}(\boldsymbol{K},\boldsymbol{K}'), & p'^2>0,\\ -\tilde{M}(\boldsymbol{K},\boldsymbol{K}'), & p'^2<0,\end{cases} \tag{3.17a}$$

$$N^\dagger(\boldsymbol{K},\boldsymbol{K}')=\begin{cases}-\tilde{M}(\boldsymbol{K},\boldsymbol{K}'), & p'^2>0,\\ -\tilde{N}(\boldsymbol{K},\boldsymbol{K}'), & p'^2<0.\end{cases} \tag{3.17b}$$

Upon taking the hermitian conjugate of eq. (3.8), we find that $V^{\dagger}(\boldsymbol{K},\boldsymbol{K}')$ satisfies

$$-\left[h_N^*(K)\,N^{\dagger}(\boldsymbol{K},\boldsymbol{K}_0)+h_M^*(K)\,M^{\dagger}(\boldsymbol{K},\boldsymbol{K}_0)\right]/2\mathrm{i}p = \sum_{\boldsymbol{K}'} V^{\dagger}(\boldsymbol{K},\boldsymbol{K}')\frac{1}{2p'}\left[N^{\dagger}(\boldsymbol{K}',\boldsymbol{K}_0)-M^{\dagger}(\boldsymbol{K}',\boldsymbol{K}_0)\right]. \tag{3.18}$$

By using (3.17) and the fact that $h_N^*(K)=h_M(K)$ for $K^2<(\omega/c)^2$, we see that $\tilde{V}(\boldsymbol{K},\boldsymbol{K}')$ satisfies the same equation as $V^{\dagger}(\boldsymbol{K},\boldsymbol{K}')$. We thus conclude that $V(\boldsymbol{K},\boldsymbol{K}')$ is hermitian if it is self-reciprocal.

It is important to note that even an approximate $V$, provided that it is hermitian and self-reciprocal, gives a unitary and self-reciprocal $S$. In particular, we can use an expansion of $V(\boldsymbol{K},\boldsymbol{K}')$ in powers of $\zeta(\boldsymbol{R})$ [11], from (3.8), because reciprocity and hermiticity hold to each other in $\zeta$. We report here the lowest order terms of that expansion,

$$V(\boldsymbol{K},\boldsymbol{K}_0)=V^{(1)}(\boldsymbol{K},\boldsymbol{K}_0)+V^{(2)}(\boldsymbol{K},\boldsymbol{K}_0)+\dots, \tag{3.19}$$

$$V^{(1)}(\boldsymbol{K},\boldsymbol{K}_0)=\zeta_{K-K_0}\left(\frac{\epsilon-1}{\epsilon}\right)\begin{pmatrix} \dfrac{\epsilon K K_0-(\hat{K}\cdot\hat{K}_0)qq_0}{\epsilon} & -\dfrac{\omega}{c}q(\hat{K}\times\hat{K}_0) \\ -\dfrac{\omega}{c}(\hat{K}\times\hat{K}_0)q_0 & \epsilon\left(\dfrac{\omega}{c}\right)^2(\hat{K}\cdot\hat{K}_0) \end{pmatrix}, \tag{3.20a}$$

$$V^{(2)}(\boldsymbol{K},\boldsymbol{K}_0)=\mathrm{i}\left(\frac{1-\epsilon}{\epsilon}\right)\frac{(\zeta^2)_{\boldsymbol{K}-\boldsymbol{K}_0}}{2} \times\begin{pmatrix} \dfrac{\left[KK_0-(\hat{K}\cdot\hat{K}_0)qq_0\right]}{\epsilon}(q+q_0) & -\left(\dfrac{\omega}{c}\right)(\hat{K}\times\hat{K}_0)q(q+q_0) \\ -\left(\dfrac{\omega}{c}\right)(\hat{K}\times\hat{K}_0)(q+q_0)q_0 & \epsilon\left(\dfrac{\omega}{c}\right)^2(\hat{K}\cdot\hat{K}_0)(q+q_0) \end{pmatrix}, \tag{3.20b}$$

$$-\mathrm{i}\left(\frac{1-\epsilon}{\epsilon}\right)^2\sum_{\boldsymbol{K}'}\zeta_{\boldsymbol{K}-\boldsymbol{K}'}\zeta_{\boldsymbol{K}'-\boldsymbol{K}_0} \times\begin{pmatrix} \dfrac{q(\hat{K}\cdot\hat{K}')q'(\hat{K}'\cdot\hat{K}_0)q_0}{\epsilon} & \left(\dfrac{\omega}{c}\right)q(\hat{K}\cdot\hat{K}')q'(\hat{K}'\times\hat{K}_0) \\ \left(\dfrac{\omega}{c}\right)(\hat{K}\times\hat{K}')q'(\hat{K}'\cdot\hat{K}_0)q_0 & \epsilon\left(\dfrac{\omega}{c}\right)^2(\hat{K}\times\hat{K}')q'(\hat{K}'\times\hat{K}_0) \end{pmatrix}. \tag{3.21}$$

We see that $V^{(1)}(\boldsymbol{K},\boldsymbol{K}')$ and $V^{(2)}(\boldsymbol{K},\boldsymbol{K}')$ are manifestly self-reciprocal and hermitian; they are obtained directly from (3.8) in this form. It turns out that $V^{(n)}(\boldsymbol{K},\boldsymbol{K}')$ for $n\geqslant 3$, as obtained from subsequent iterations of (3.8), are not manifestly hermitian and self-reciprocal, although, order by order, $V^{(n)} - \tilde{V}^{(n)}$ can be shown to vanish with the aid of identities derived from (3.11). One can use the expression $(V^{(n)} + \tilde{V}^{(n)})/2$, which is manifestly self-reciprocal and hermitian at the cost, however, of adding more terms.

The perturbative formulae (3.20) and (3.21), in conjunction with the exact equations (3.2) and (3.3), represent the main results of this paper. They reduce the boundary value problem, in the presence of surface resonances, to a two-dimensional scattering problem with an effective potential $V$.

## Appendix A

In order to evaluate the vector products in eq. (2.11), we need an expression for the vector $\boldsymbol{n}$ that is normal to the corrugated surface specified by the equation

$$z - \zeta(\boldsymbol{R}) = 0. \tag{A.1}$$

The normal direction is given by the gradient

$$\boldsymbol{n} = \hat{z} - \nabla\zeta(\boldsymbol{R}), \quad \text{where} \quad \nabla = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y}. \tag{A.2}$$

The differential element of surface area, $\mathrm{d}S$, may be expressed as

$$\mathrm{d}S = \frac{\mathrm{d}^2R}{(\hat{n}\cdot\hat{z})} = |\boldsymbol{n}|\,\mathrm{d}^2R. \tag{A.3}$$

Therefore in (2.11) we may make the replacement

$$\hat{n}\,\mathrm{d}S = \boldsymbol{n}\,\mathrm{d}^2R, \tag{A.4}$$

with $\boldsymbol{n}$ given by (A.2). Because the normal vector appears in the integrand of expression (2.11), we will need to evaluate the integral

$$\int \mathrm{d}^2R\,[\nabla\zeta(\boldsymbol{R})]\,\mathrm{e}^{\mathrm{i}(\boldsymbol{K}'-\boldsymbol{K})\cdot\boldsymbol{R}}\,\mathrm{e}^{\mathrm{i}(p'-q)\zeta(\boldsymbol{R})} = \int \mathrm{d}^2R\,\mathrm{e}^{\mathrm{i}(\boldsymbol{K}'-\boldsymbol{K})\cdot\boldsymbol{R}}\,\frac{\nabla(\mathrm{e}^{\mathrm{i}(p'-q)\zeta(\boldsymbol{R})})}{\mathrm{i}(p'-q)}. \tag{A.5a}$$

Integrating this by parts gives

$$\int \mathrm{d}^2R\,\frac{\mathrm{e}^{\mathrm{i}(p'-q)\zeta(\boldsymbol{R})}}{\mathrm{i}(p'-q)}\,\nabla(\mathrm{e}^{\mathrm{i}(\boldsymbol{K}'-\boldsymbol{K})\cdot\boldsymbol{R}}) = \frac{\boldsymbol{K}-\boldsymbol{K}'}{p'-q}\int \mathrm{d}^2R\,\mathrm{e}^{\mathrm{i}(\boldsymbol{K}'-\boldsymbol{K})\cdot\boldsymbol{R}}\,\mathrm{e}^{\mathrm{i}(p'-q)\zeta(\boldsymbol{R})}. \tag{A.5b}$$

Therefore in the integrand we can make the replacement

$$\nabla\zeta \to \frac{\boldsymbol{K}-\boldsymbol{K}'}{p'-q}, \tag{A.6}$$

$$\boldsymbol{n} = \frac{\boldsymbol{K}'-\boldsymbol{K}}{p'-q} + \hat{z}. \tag{A.7}$$

In terms of the propagation vectors, $\boldsymbol{k}' = \boldsymbol{K}' + p'\hat{z}$ and $\boldsymbol{k}_\epsilon = \boldsymbol{K} + q\hat{z}$, the normal vector (A.7) is

$$\boldsymbol{n} = \frac{\boldsymbol{K}' - \boldsymbol{K}_\epsilon}{p' - q}. \tag{A.8}$$

The vector products appearing in expression (2.13) now become

$$\mathrm{i}\boldsymbol{n} \times (\mathrm{i}\boldsymbol{k}' \times \boldsymbol{E}^{>}(\boldsymbol{k}')) = \frac{-\mathrm{i}}{p' - q}[(\boldsymbol{k}_\epsilon - \boldsymbol{k}')\cdot \boldsymbol{E}^{>}(\boldsymbol{k}')\boldsymbol{k}' - (\boldsymbol{k}_\epsilon - \boldsymbol{k}')\cdot \boldsymbol{k}'\boldsymbol{E}^{>}(\boldsymbol{k}')], \tag{A.9a}$$

$$-(\boldsymbol{n} \times \boldsymbol{E}^{>}(\boldsymbol{k}')) \times \mathrm{i}\boldsymbol{k}_\epsilon = \frac{\mathrm{i}}{p' - q}[(\boldsymbol{k}_\epsilon - \boldsymbol{k}')\cdot \boldsymbol{k}_\epsilon \boldsymbol{E}^{>}(\boldsymbol{k}') - \boldsymbol{E}^{>}(\boldsymbol{k}')\cdot \boldsymbol{k}_\epsilon(\boldsymbol{k}_\epsilon - \boldsymbol{k}')], \tag{A.9b}$$

$$\frac{-\boldsymbol{n}\cdot \boldsymbol{E}^{>}(\boldsymbol{k}')}{\epsilon}\mathrm{i}\boldsymbol{k}_\epsilon = \frac{\mathrm{i}}{\epsilon(p' - q)}(\boldsymbol{k}_\epsilon - \boldsymbol{k}')\cdot \boldsymbol{E}^{>}(\boldsymbol{k}')\boldsymbol{k}_\epsilon. \tag{A.9c}$$

Because the $E$ field is transverse, $\boldsymbol{E}^{>}(\boldsymbol{k}')\cdot \boldsymbol{k}' = 0$. The sum of these terms then becomes

$$\frac{-\mathrm{i}}{p' - q}\left[(k'^2 - k_\epsilon^2)\boldsymbol{E}^{>}(\boldsymbol{k}') + \left(1 - \frac{1}{\epsilon}\right)\boldsymbol{k}_\epsilon \cdot \boldsymbol{E}^{>}(\boldsymbol{k}')\boldsymbol{k}_\epsilon\right]$$
$$= \frac{\mathrm{i}(\epsilon - 1)}{p' - q}\left[\left(\frac{\omega}{c}\right)^2 \boldsymbol{E}^{>}(\boldsymbol{k}') - \frac{\boldsymbol{k}_\epsilon}{\epsilon}\boldsymbol{k}_\epsilon \cdot \boldsymbol{E}^{>}(\boldsymbol{k}')\right]. \tag{A.10}$$

## Appendix B

In eq. (3.11c), using $p'^2 = (\omega/c)^2 - K'^2$ and the fact that $(\hat{K}\cdot\hat{K}')(\hat{K}' \times \hat{K}_0)_z + (\hat{K} \times \hat{K}')_z(\hat{K}'\cdot\hat{K}_0) = (\hat{K} \times \hat{K}_0)_z$, we obtain

$$\int \mathrm{d}^2R_1\,\mathrm{d}^2R_2 \sum_{\boldsymbol{K}'} \frac{1}{p'}\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{K}-\boldsymbol{K}')\cdot \boldsymbol{R}_1}\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{K}'-\boldsymbol{K}_0)\cdot \boldsymbol{R}_2}\,\mathrm{e}^{-\mathrm{i}[q\zeta(\boldsymbol{R}_1)+q_0\zeta(\boldsymbol{R}_2)]}$$
$$\times\left[\mathrm{e}^{\mathrm{i}p'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]}\left(\frac{(\boldsymbol{K}' \times \hat{\boldsymbol{K}}_0)_z[q(\hat{\boldsymbol{K}}\cdot \boldsymbol{K}') - Kp'] - q(\omega/c)^2(\hat{\boldsymbol{K}} \times \hat{\boldsymbol{K}}_0)_z}{(q - p')(q_0 + p')}\right)\right.$$
$$\left.-\mathrm{e}^{-\mathrm{i}p'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]}\left(\frac{(\boldsymbol{K}' \times \hat{\boldsymbol{K}}_0)_z[q(\hat{\boldsymbol{K}}\cdot \boldsymbol{K}') + Kp'] - q(\omega/c)^2(\hat{\boldsymbol{K}} \times \hat{\boldsymbol{K}}_0)_z}{(q + p')(q_0 - p')}\right)\right]$$
$$= 0. \tag{B.1}$$

In the first term we can make the following replacements:

$$\boldsymbol{K}' = \boldsymbol{K} - (\boldsymbol{K} - \boldsymbol{K}') \to \boldsymbol{K} + (q - p')\nabla\zeta(\boldsymbol{R}_1), \tag{B.2a}$$

$$\boldsymbol{K}' = \boldsymbol{K}_0 + (\boldsymbol{K}' - \boldsymbol{K}_0) \to \boldsymbol{K}_0 - (q_0 + p')\nabla\zeta(\boldsymbol{R}_2), \tag{B.2b}$$

which are found by performing an integration by parts. The second term is handled in the same way; we then find

$$\frac{(\boldsymbol{K}'\times\hat{\boldsymbol{K}}_0)_z[q(\hat{\boldsymbol{K}}\cdot\boldsymbol{K}')\mp Kp']}{(q\mp p')(q_0\pm p')}\to -[\nabla\zeta(\boldsymbol{R}_2)\times\hat{\boldsymbol{K}}_0]_z[K+q\hat{\boldsymbol{K}}\cdot\nabla\zeta(\boldsymbol{R}_1)].$$

Eq. (B.1) will be satisfied provided

$$\int d^2R_1\, d^2R_2\, e^{-i[q\zeta(\boldsymbol{R}_1)+q_0\zeta(\boldsymbol{R}_2)]}[\nabla\zeta(\boldsymbol{R}_2)\times\hat{\boldsymbol{K}}_0]_z[K+q\hat{\boldsymbol{K}}\cdot\nabla\zeta(\boldsymbol{R}_1)]$$
$$\times\sum_{\boldsymbol{K}'}e^{-i(\boldsymbol{K}-\boldsymbol{K}')\cdot\boldsymbol{R}_1}e^{-i(\boldsymbol{K}'-\boldsymbol{K}_0)\cdot\boldsymbol{R}_2}\frac{\sin\{p'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]\}}{p'} \tag{B.3}$$

and

$$\int d^2R_1\, d^2R_2\, e^{-i[q\zeta(\boldsymbol{R}_1)+q_0\zeta(\boldsymbol{R}_2)]}\sum_{\boldsymbol{K}'}e^{-i(\boldsymbol{K}-\boldsymbol{K}')\cdot\boldsymbol{R}_1}e^{-i(\boldsymbol{K}'-\boldsymbol{K}_0)\cdot\boldsymbol{R}_2}$$
$$\times\left(\frac{e^{ip'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]}}{(q-p')(q_0+p')}-\frac{e^{-ip'[\zeta(\boldsymbol{R}_1)-\zeta(\boldsymbol{R}_2)]}}{(q+p')(q_0-p')}\right) \tag{B.4}$$

both vanish. It has already been shown that the one-dimensional analogs of (B.3) and (B.4) are zero [10,12], and the method of proof can be extended to the two-dimensional case trivially; hence, (3.11c) is satisfied.

Similarly, in (3.11b), the terms involving the unit vectors become

$$-(q\mp p')(q_0\pm p')[\hat{\boldsymbol{K}}\times\nabla\zeta(\boldsymbol{R}_1)]\cdot[\nabla\zeta(\boldsymbol{R}_2)\times\hat{\boldsymbol{K}}_0]-(\omega/c)^2(\hat{\boldsymbol{K}}\cdot\hat{\boldsymbol{K}}_0).$$
$$=-(\hat{\boldsymbol{K}}\times\boldsymbol{K}')\cdot(\boldsymbol{K}'\times\hat{\boldsymbol{K}}_0)-(\omega/c)^2(\hat{\boldsymbol{K}}\cdot\hat{\boldsymbol{K}}_0). \tag{B.5}$$

Using replacements such as (B.2), (B.5) becomes

$$-(q\mp p')(q_0\pm p')[\hat{\boldsymbol{K}}\times\nabla\zeta(\boldsymbol{R}_1)]\cdot[\nabla\zeta(\boldsymbol{R}_2)\times\hat{\boldsymbol{K}}_0]-(\omega/c)^2(\hat{\boldsymbol{K}}\cdot\hat{\boldsymbol{K}}_0).$$

We again obtain expressions like (B.3) and (B.4) which we know vanish, and thus (3.11b) is satisfied.

In (3.11a), we multiply out the factors in brackets; using the summation of unit vector products in (B.5), the set of factors that multiply $F^+(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')$ becomes

$$KK_0K'^2+qq_0(\hat{\boldsymbol{K}}\cdot\boldsymbol{K}')(\boldsymbol{K}'\cdot\hat{\boldsymbol{K}}_0)+p'qK_0(\hat{\boldsymbol{K}}\cdot\boldsymbol{K}')$$
$$-p'q_0K(\hat{\boldsymbol{K}}_0\cdot\boldsymbol{K}')-(\omega/c)^2(\hat{\boldsymbol{K}}\cdot\hat{\boldsymbol{K}}_0). \tag{B.6}$$

In the process of proving (3.11b) we also proved (cf. (B.5)) that

$$qq_0\sum_{\boldsymbol{K}'}\frac{1}{p'}[F^+(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')+F^-(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')][(\hat{\boldsymbol{K}}\times\boldsymbol{K}')\cdot(\boldsymbol{K}'\times\hat{\boldsymbol{K}}_0)]$$

vanishes; hence we may subtract this from (3.11a). When the additional terms are combined with (B.6) we obtain

$$KK_0K'^2 - p'^2qq_0(\hat{K}\cdot\hat{K}_0) + p'qK_0(\hat{K}\cdot\boldsymbol{K}') - p'q_0K(\hat{K}_0\cdot\boldsymbol{K}')$$
$$= [K\boldsymbol{K}' + p'q\hat{K}]\cdot[\boldsymbol{K}'K_0 - p'q_0\hat{K}_0]. \tag{B.7}$$

Using $q^2 + K^2 = \epsilon\omega^2/c^2$ and (B.2),

$$[K\boldsymbol{K}' + p'q\hat{K}] \to \{K[\boldsymbol{K} + (q-p')\nabla\zeta(\boldsymbol{R}_1)]$$
$$-(q-p')q\hat{K} + [\epsilon(\omega/c)^2 - K^2]\hat{K}\}, \tag{B.8}$$

from which we obtain (after performing the analogous operation on $\boldsymbol{K}'K_0 - p'q_0\hat{K}_0$)

$$\frac{K\boldsymbol{K}' + p'q\hat{K}}{q-p'} \to \hat{K}\left(\frac{\epsilon(\omega/c)^2}{q-p'} - q\right) + K\nabla\zeta(\boldsymbol{R}_1), \tag{B.9a}$$

$$\frac{K_0\boldsymbol{K}' - p'q\hat{K}_0}{q_0+p'} \to \hat{K}_0\left(\frac{\epsilon(\omega/c)^2}{q_0+p'} - q_0\right) - K_0\nabla\zeta(\boldsymbol{R}_2). \tag{B.9b}$$

As a result,

$$\frac{[K\boldsymbol{K}' + p'q\hat{K}]\cdot[K_0\boldsymbol{K}' - p'q_0\hat{K}_0]}{(q-p')(q_0+p')}$$
$$\to \frac{(\hat{K}\cdot\hat{K}_0)[\epsilon(\omega/c)^2]}{(q-p')(q_0+p')} + [\hat{K}q - K\nabla\zeta(\boldsymbol{R}_1)]\cdot[\hat{K}_0q_0 + K_0\nabla\zeta(\boldsymbol{R}_2)]$$
$$-\epsilon\left(\frac{\omega}{c}\right)^2\left(\frac{\hat{K}\cdot[q_0\hat{K}_0 + K_0\nabla\zeta(\boldsymbol{R}_2)]}{q-p'} + \frac{\hat{K}_0\cdot[q\hat{K} - K\nabla\zeta(\boldsymbol{R}_1)]}{q_0+p'}\right). \tag{B.10}$$

By performing an integration by parts we also have the following identities [10]

$$\frac{(\epsilon-1)(\omega/c)^2}{q-p'} \to q + p' - (\boldsymbol{K}+\boldsymbol{K}')\cdot\nabla\zeta(\boldsymbol{R}_1), \tag{B.11a}$$

$$\frac{(\epsilon-1)(\omega/c)^2}{q_0+p'} \to q_0 - p' + (\boldsymbol{K}_0+\boldsymbol{K}')\cdot\nabla\zeta(\boldsymbol{R}_2), \tag{B.11b}$$

and, using $p'^2 + K'^2 = (\omega/c)^2$:

$$p' - \boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_1) \to \frac{(\omega/c)^2 - \boldsymbol{K}\cdot\boldsymbol{K}' - q\boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_1)}{p'},$$

$$p' - \boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_2) \to \frac{(\omega/c)^2 - \boldsymbol{K}_0\cdot\boldsymbol{K}' + q_0\boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_2)}{p'}.$$

When (B.11) and (B.12) are substituted into (B.10), we obtain finally

$$\left[\frac{KK'+p'q\hat{K}}{q-p'}\right]\cdot\left[\frac{K_0K'-p'q_0\hat{K}_0}{q_0+p'}\right]\to\frac{\left[\epsilon(\omega/c)^2\right]^2(\hat{K}\cdot\hat{K}_0)}{(q-p')(q_0+p')}$$
$$+\left[\hat{K}q-K\nabla\zeta(\boldsymbol{R}_1)\right]\cdot\left[\hat{K}_0q_0+K_0\nabla\zeta(\boldsymbol{R}_2)\right]$$
$$-\frac{\epsilon}{\epsilon-1}\left(\left[(\hat{K}\cdot\hat{K}_0)q-K\hat{K}_0\cdot\nabla\zeta(\boldsymbol{R}_1)\right]\left[q_0+\boldsymbol{K}_0\cdot\nabla\zeta(\boldsymbol{R}_2)\right]\right.$$
$$\left.+\left[(\hat{K}\cdot\hat{K}_0)q_0+K_0\hat{K}\cdot\nabla\zeta(\boldsymbol{R}_2)\right]\left[q-\boldsymbol{K}\cdot\nabla\zeta(\boldsymbol{R}_1)\right]\right)$$
$$+\frac{\epsilon}{\epsilon-1}\frac{1}{p'}\left(\left[(\hat{K}\cdot\hat{K}_0)q-K\hat{K}_0\cdot\nabla\zeta(\boldsymbol{R}_1)\right]\left[(\omega/c)^2-\boldsymbol{K}'\cdot\boldsymbol{K}_0+q_0\boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_2)\right]\right.$$
$$\left.-\left[(\hat{K}\cdot\hat{K}_0)q_0+K_0\hat{K}\cdot\nabla\zeta(\boldsymbol{R}_2)\right]\left[(\omega/c)^2-\boldsymbol{K}'\cdot\boldsymbol{K}-q\boldsymbol{K}'\cdot\nabla\zeta(\boldsymbol{R}_1)\right]\right).\quad\text{(B.13)}$$

The factors analogous to (B.13) which multiply $F^-(\boldsymbol{K},\boldsymbol{K}_0,\boldsymbol{K}')$ may be obtained from (B.13) by letting $\boldsymbol{K}\to-\boldsymbol{K}_0$, $\boldsymbol{K}_0\to-\boldsymbol{K}$, $\boldsymbol{R}_1\to\boldsymbol{R}_2$, and $\boldsymbol{K}'\to-\boldsymbol{K}'$. We have now obtained from (3.11a) an expression which generalizes a condition obtained previously for the reciprocity of p-wave scattering from a one-dimensional profile [10]. The proof proceeds from here in the same way, and it follows that $V=\tilde{V}$.

## Appendix C

We shall prove that the unitarity condition (3.16) follows from the $T$-matrix equation (3.3b) if $V$ is hermitian. First, using (3.15b), we rewrite (3.16) as

$$f(K)\,T(\boldsymbol{K},\boldsymbol{K}_0)\,f^*(K_0)-f^*(K_0)\,T^*(\boldsymbol{K}_0,\boldsymbol{K})\,f(K)$$
$$=\sum_{K'<(\omega/c)}f^*(K')\,T^*(\boldsymbol{K}',\boldsymbol{K})\,f(K)\,2\mathrm{i}p'f(K')\,T(\boldsymbol{K}',\boldsymbol{K}_0)\,f^*(K_0).\quad\text{(C.1)}$$

This suggests that we work with the matrix

$$T'=fTf^\dagger.\quad\text{(C.2)}$$

We thus begin by rewriting (3.3b) as

$$T'=V'+T'G'V',\quad\text{(C.3)}$$

where $G'=(f^\dagger)^{-1}Gf^{-1}$. We see that if $V=V^\dagger$, then $V'=V'^\dagger$, and (C.3) leads to the well known result [13]

$$T'-T'^\dagger=T^\dagger(G-G^\dagger)T.\quad\text{(C.4)}$$

When (C.4) is written out in detail, it becomes

$$f(K)\,T(\boldsymbol{K},\boldsymbol{K}_0)\,f^*(K_0)-f^*(K_0)\,T^*(\boldsymbol{K}_0,\boldsymbol{K})\,f(K)$$
$$=\sum_{\boldsymbol{K}'} f^*(K')\,T^*(\boldsymbol{K}',\boldsymbol{K})\,f(K)$$
$$\times\{|f(K')|^{-2}[G(K')-G^*(K')]\}\,f(K')\,T(\boldsymbol{K}',\boldsymbol{K}_0)\,f^*(K_0). \tag{C.5}$$

By using the forms for $f(K')$ and $G(K')$ (eqs. (3.4b) and (3.4c)), we find that the quantity in brackets reduces to

$$|f(K')|^{-2}[G(K')-G^*(K')]=2\mathrm{i}\,\mathrm{Re}\,p'. \tag{C.6}$$

The sum over $\boldsymbol{K}'$ in (C.5) is thus restricted to open channels, and (C.5) is equivalent to (C.1).

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