Integral equation treatment of scattering from rough surfaces

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A self-consistent integral equation describing scattering from rough surfaces is obtained. This integral equation automatically takes into account the discontinuous behavior of the zeroth-order fields and Green's functions and leads to results for various scattering and extinction cross sections in agreement with the results obtained by other methods such as those based on the extinction theorem and the Rayleigh-Fano method.

A number of treatments of scattering from rough surfaces have appeared recently.[1–6] The results of different calculations agree with each other only partially. Some of the differences in the results have been properly explained[2–6] while others still persist. For example, the method, used by the present author,[5] based on the Ewald-Oseen extinction theorem leads to results in perfect agreement with those of Marvin, Toigo, and Celli.[4] The latter authors used Rayleigh-Fano type of perturbation theory. In an earlier paper Maradudin and Mills[3] used an integral-equation formulation to study scattering from rough surfaces. Some of their results concerning p-p scattering are in disagreement with those obtained by other methods. In this paper we discuss how the integral equation involving rough surfaces has to be obtained from Maxwell equations by proper application of Green's theorem to different domains and by properly identifying the zeroth-order fields.[7] We show that this self-consistent integral equation leads to results for first-order reflected and transmitted fields in agreement with those of Juranek, Agarwal, Marvin, Toigo, and Celli.

For simplicity we deal with an isotropic homogeneous medium. Maxwell's equations can be used to show that the electric field $\vec{E}$ obeys the equation

$$\nabla\times\nabla\times\vec{E}-(\omega^2/c^2)[\epsilon\eta(\rho)+\eta(-\rho)]\vec{E}=0\,, \qquad (1)$$

where we assume that the medium occupies the domain $\rho\geq 0$ and the region $\rho<0$ is the vacuum region. The surface of the medium is characterized by $\rho=0$. Let $\rho_0=0$ be the smooth surface corresponding to the rough surface $\rho=0$. We now introduce the exact Green's function which is the solution

$$\nabla\times\nabla\times\overleftrightarrow{G}-(\omega^2/c^2)[\epsilon\eta(\rho_0)+\eta(-\rho_0)]\overleftrightarrow{G}=4\pi\delta(\vec{r}-\vec{r}\,')\overleftrightarrow{I}\,, \qquad (2)$$

subject to the usual boundary conditions at $\rho_0=0$ and outgoing boundary conditions at infinity.

In the region V occupied by the medium $\overleftrightarrow{G}$ obeys

$$\nabla\times\nabla\times\overleftrightarrow{G}-(\omega^2/c^2)\epsilon\overleftrightarrow{G}=4\pi\delta(\vec{r}-\vec{r}\,')\overleftrightarrow{I}-(\omega^2/c^2)\eta(\rho)\eta(-\rho_0)(\epsilon-1)\overleftrightarrow{G}\,, \qquad (3)$$

and outside V the equation for $\overleftrightarrow{G}$ can be written

$$\nabla\times\nabla\times\overleftrightarrow{G}-(\omega^2/c^2)\overleftrightarrow{G}=4\pi\delta(\vec{r}-\vec{r}\,')\overleftrightarrow{I}+(\omega^2/c^2)\eta(-\rho)\eta(\rho_0)(\epsilon-1)\overleftrightarrow{G}\,. \qquad (4)$$

We now apply the vectorial form of the Green's theorem over a volume V' in which the fields are continuous, then

$$\int_{V'}\vec{E}(\vec{r}\,')\delta(\vec{r}-\vec{r}\,')\,d^3r'=-\tfrac{1}{4}\pi\Sigma(\vec{r})+\int_{V'}\vec{E}(\vec{r}\,')\overleftrightarrow{Q}(\vec{r}\,',\vec{r})\,d^3r'\,, \qquad (5)$$

where

$$-4\pi\overleftrightarrow{Q}=-(\omega^2/c^2)(\epsilon-1)\overleftrightarrow{G}[\eta(\rho)\eta(-\rho_0)-\eta(-\rho)\eta(\rho_0)]\,, \qquad (6)$$

$$\Sigma(\vec{r})=\int_{S'}[\vec{n}\,'\times\vec{\nabla}'\times\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,',\vec{r})+\vec{n}\,'\times\vec{E}(\vec{r}\,')\cdot\vec{\nabla}'\times\overleftrightarrow{G}(\vec{r}\,',\vec{r})]\,dS\,, \qquad (7)$$

and where $\vec{n}\,'$ is the unit outward normal to the surface S. We now apply the identity (5) to four cases—the ones in which V is taken to coincide with the scattering volume V ($\rho>0$), vacuum $\tilde{V}$ ($\rho<0$) and by taking, respectively, $\vec{r}$ inside and outside the volume under consideration. In this manner we obtain following equations:

$\vec{r}\in V,\ \vec{r}\,'\in V$:

$$\vec{E}(\vec{r}_>)=-(1/4\pi)\Sigma^{(+)}(\vec{r}_>)+(1/4\pi)(\epsilon-1)\frac{\omega^2}{c^2}\int\eta(\rho)\times\eta(-\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,',\vec{r}_>)\,d^3r'\,, \qquad (8)$$

$\vec{r}\in V,\ \vec{r}\,'\in\tilde{V}$:

$$0=(1/4\pi)\Sigma^{(-)}(\vec{r}_>)-(1/4\pi)\Sigma^{(\infty)}(\vec{r}_>)-(1/4\pi)(\epsilon-1)\times\frac{\omega^2}{c^2}\int\eta(-\rho)\eta(\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,',\vec{r}_>)\,d^3r'\,, \qquad (9)$$

$\vec{r}\in\tilde{V},\ \vec{r}\,'\in\tilde{V}$:

$$\vec{E}(\vec{r}_<)=(1/4\pi)\Sigma^{(-)}(\vec{r}_<)-(1/4\pi)\Sigma^{(\infty)}(\vec{r}_<)-(1/4\pi)(\epsilon-1)$$

$$\times \frac{\omega^2}{c^2} \int \eta(-\rho)\eta(\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_<)\, d^3r' , \quad (10)$$

$\vec{r}\in\tilde{V}$. $\vec{r}\,'\in V$:

$$0 = -(1/4\pi)\Sigma^{(+)}(\vec{r}_<) + (1/4\pi)(\epsilon - 1)\frac{\omega^2}{c^2}\int \eta(\rho) \times \eta(-\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_<)\, d^3r' , \quad (11)$$

where

$$\Sigma^{(\pm)}(\vec{r}) = \int_{S^\pm} dS[\vec{n}\times\vec{\nabla}'\times\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}) + \vec{n}\times\vec{E}(\vec{r}\,')\cdot\vec{\nabla}'\times\overleftrightarrow{G}(\vec{r}\,', \vec{r})] , \quad (12)$$

and where $\vec{n}$ is the unit normal to the surface $\rho = 0$ pointing from the medium to the vacuum region. The superscripts + (−) means that the values should be taken at $\rho = 0^+ (0^-)$. $\Sigma^{(\infty)}$ is the contribution from the surface at infinity. It should be noted that the surface integrals involve the tangential components of the electric and magnetic field, which are continuous across the dielectric interface. Similarly the tangential components of $\overleftrightarrow{G}$ and $\vec{\nabla}\times\overleftrightarrow{G}$ are continuous across $\rho_0 = 0$. When the surfaces $\rho = 0$ and $\rho_0 = 0$ do not coincide, then the continuity conditions also hold because as far as $\overleftrightarrow{G}$ is concerned $\rho = 0$ is only some artificial surface and hence we get

$$\Sigma^{(+)}(\vec{r}_{\gtrless}) = \Sigma^{(-)}(\vec{r}_{\gtrless}) . \quad (13)$$

$\Sigma^{(\infty)}$ is seen to represent the zeroth-order fields, for in the absence of any roughness ($\rho \equiv \rho_0$)

$$\vec{E}(\vec{r}_>) = \vec{E}^{(0)}(\vec{r}_>) = -(1/4\pi)\Sigma^{(+)}(\vec{r}_>) = -(1/4\pi)\Sigma^{(-)}(\vec{r}_>) = -(1/4\pi)\Sigma^{(\infty)}(\vec{r}_>)$$

and thus we can identify[8]

$$-(1/4\pi)\Sigma^{(\infty)}(\vec{r}_{\gtrless}) = \vec{E}^{(0)}(\vec{r}_{\gtrless}) . \quad (14)$$

On combining (8)–(11), (13), and (14) we obtain the following integral equation:

$$\vec{E}(\vec{r}_{\gtrless}) = \vec{E}^{(0)}(\vec{r}_{\gtrless}) + (1/4\pi)(\epsilon - 1)\frac{\omega^2}{c^2}\int d^3r' \times[\eta(\rho)\eta(-\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_{\gtrless}) - \eta(-\rho)\eta(\rho_0)\vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_{\gtrless})] . \quad (15)$$

It is clear from the derivation of the integral equation that in the first term (second term) in (15), $\vec{E}$ is the field inside (outside) the medium and the Green's function G is at points such that $\rho_0 < 0$ ($\rho_0 > 0$). This difference is important when one is doing the perturbation calculation with (15). This is our final integral equation which we will apply for the case of roughness on a perfectly flat surface, i.e., for the case when the rough surface is described by $\rho \equiv z + hf(x, y) = 0$ and the flat surface by $z = 0$. Then (15) becomes

$$\vec{E}(\vec{r}_{\gtrless}) = \vec{E}^{(0)}(\vec{r}_{\gtrless}) + (1/4\pi)(\epsilon - 1)\frac{\omega^2}{c^2}\iint_{-\infty}^{+\infty} dx'\, dy' \times[\eta(hf)\mathcal{I}_1 + \eta(-hf)\mathcal{I}_2] , \quad (16)$$

where

$$\mathcal{I}_1 = \int_{-hf}^{0} dz'\, \vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_{\gtrless}) , \quad (17)$$

$$\mathcal{I}_2 = -\int_{0}^{-hf} dz'\, \vec{E}(\vec{r}\,')\cdot\overleftrightarrow{G}(\vec{r}\,', \vec{r}_{\gtrless}) . \quad (18)$$

It is clear from the structure of $\mathcal{I}_1$, $\mathcal{I}_2$, that these are at least of first order in h and hence to lowest order in h we can write, in view of our remarks following Eq. (15),

$$\mathcal{I}_1 = hf(x', y')\vec{E}^{(0)}(x', y', 0^+)\cdot\overleftrightarrow{G}(x', y', 0^-; \vec{r}_{\gtrless}) , \quad (19)$$

$$\mathcal{I}_2 = hf(x', y')\vec{E}^{(0)}(x', y', 0^-)\cdot\overleftrightarrow{G}(x', y', 0^+; \vec{r}_{\gtrless}) . \quad (20)$$

Now using the boundary conditions

$$E_i^{(0)}(x', y', 0^+) = E_i^{(0)}(x', y', 0^-) , \qquad i = 1, 2 ,$$

$$E_3^{(0)}(x', y', 0^-) = \epsilon E_3^{(0)}(x', y', 0^+) ,$$

$$G_{ij}(x', y', 0^-; \vec{r}_{\gtrless}) = G_{ij}(x', y', 0^+; \vec{r}_{\gtrless}) , \quad i = 1, 2 ;$$

$$G_{3j}(x', y', 0^-; \vec{r}_{\gtrless}) = \epsilon G_{3j}(x', y', 0^+; \vec{r}_{\gtrless}) , \quad (21)$$

we get

$$\mathcal{I}_1 = \mathcal{I}_2 = hf(x', y')[\vec{E}_{\parallel}^{(0)}(x', y', 0^+)\cdot\overleftrightarrow{G}(x', y', 0^+; \vec{r}_{\gtrless}) + \epsilon E_z^{(0)}(x', y', 0^+)\hat{z}\cdot\overleftrightarrow{G}(x', y', 0^+; \vec{r}_{\gtrless}] , \quad (22)$$

which on substituting in (16) yields

$$\vec{E}(\vec{r}_{\gtrless}) = \vec{E}^{(0)}(\vec{r}_{\gtrless}) + h\vec{E}^{(1)}(\vec{r}_{\gtrless}) , \quad (23)$$

$$\vec{E}^{(1)}(\vec{r}_>) = \int d^2\kappa\, \vec{\mathcal{E}}_T^{(1)}(\vec{\kappa})\, e^{i\vec{K}\cdot\vec{r}} ,$$

$$\vec{E}^{(1)}(\vec{r}_<) = \int d^2\kappa\, \vec{\mathcal{E}}_R^{(1)}(\vec{\kappa})\, e^{i\vec{K}_0'\cdot\vec{r}} ,$$

$$\vec{K} = (\vec{\kappa}, W) , \quad \vec{K}_0' = (\vec{\kappa}, -W_0) ,$$

$$W^2 = k_0^2\epsilon - \kappa^2 , \quad W_0^2 = k_0^2 - \kappa^2 , \quad (24)$$

with

$$\vec{\mathcal{E}}_T^{(1)}(\vec{\kappa}) = \pi F(\vec{\kappa} - \vec{\kappa}^{(0)})(\epsilon - 1)k_0^2[\vec{\mathcal{E}}_{T\parallel}^{(0)}\cdot\overleftrightarrow{G}(-\vec{\kappa}) + \epsilon\mathcal{E}_{Tz}^{(0)}\hat{z}\cdot\overleftrightarrow{G}(-\vec{\kappa})] , \quad (25)$$

$$\vec{\mathcal{E}}_R^{(1)}(\vec{\kappa}) = \pi F(\vec{\kappa} - \vec{\kappa}^{(0)})(\epsilon - 1)k_0^2[\vec{\mathcal{E}}_{T\parallel}^{(0)}\cdot\overleftrightarrow{g}(-\vec{\kappa}) + \mathcal{E}_{Tz}^{(0)}\hat{z}\cdot\overleftrightarrow{g}(-\vec{\kappa})] . \quad (26)$$

In deriving (25) and (26) we have assumed that the incident field was a plane wave characterized by $\vec{\kappa}^{(0)}$, $W_0^{(0)}$ $[W_0^{(0)} = (k_0^2 - \kappa^{(0)2})^{1/2}]$, $\vec{E}^{\text{inc}}(\vec{r}) = \vec{\mathcal{E}}^{(i)} \times \exp[i\vec{\kappa}^{(0)}\cdot\vec{r} + iW_0^{(0)}z]$, and that $\vec{\mathcal{E}}_T^{(0)}$ represents the zeroth-order transmitted field. The functions $\overleftrightarrow{G}(\vec{\kappa})$, $\overleftrightarrow{g}(\vec{\kappa})$ are defined by

$$\overleftrightarrow{G}(\vec{r}', \vec{r}_>) = \iint d^2\kappa\, \overleftrightarrow{G}(\vec{\kappa}) \exp[i\vec{\kappa}\cdot(\vec{r}' - \vec{r}_>) + iWz_>] ,$$

$$z' = 0^+ , \tag{27}$$

$$\overleftrightarrow{G}(\vec{r}', \vec{r}_<) = \iint d^2\kappa\, \overleftrightarrow{g}(\vec{\kappa}) \exp[i\vec{\kappa}\cdot(\vec{r}' - \vec{r}_<) - iW_0 z_<] ,$$

$$z' = 0^- . \tag{28}$$

The explicit expressions for $\vec{\mathcal{E}}_T^{(1)}$ and $\vec{\mathcal{E}}_R^{(1)}$ can be obtained by substituting[9] $\overleftrightarrow{G}(\vec{\kappa})$, $\overleftrightarrow{g}(\vec{\kappa})$. The final results are

$$\vec{\mathcal{E}}_T^{(1)}(\vec{\kappa}) = -i(\epsilon - 1)F(\vec{\kappa} - \vec{\kappa}^{(0)})[\vec{K}_0(W_0\epsilon + W)^{-1} \times (\vec{K}\cdot\vec{\mathcal{E}}_T^{(0)}) - k_0^2(W + W_0)^{-1}\vec{\mathcal{E}}_T^{(0)}] , \tag{29}$$

$$\vec{\mathcal{E}}_R^{(1)}(\vec{\kappa}) = i(\epsilon - 1)F(\vec{\kappa} - \vec{\kappa}^{(0)})(W_0\epsilon + W)^{-1} \times[(\kappa^2 + WW_0)\vec{\mathcal{E}}_{T\parallel}^{(0)} - \vec{K}'(\vec{\kappa}\cdot\vec{\mathcal{E}}_T^{(0)}) + \epsilon\mathcal{E}_{Tz}^{(0)}(W_0\vec{\kappa} + \hat{z}\kappa^2)] , \quad \vec{K}' = (\vec{\kappa}, -W) . \tag{30}$$

The results (29) and (30) are in agreement with the results obtained in the author's work [Ref. 5, Eqs. (14) and (15)], where a perturbation treatment using the Ewald-Oseen extinction theorem was given. We have checked that (29) and (30) are in agreement with the results obtained by the boundary matching method.[4,6] Since (29) and (30) are used to calculate the extinction and scattering cross sections, we have verified that the integral equation of the present paper leads to results in agreement with those obtained by other methods.

We close the paper by some remarks on the integral equation

$$\vec{E}(\vec{r}_{\gtrless}) = \vec{E}^{(0)}(\vec{r}_{\gtrless}) + (1/4\pi)\frac{\omega^2}{c^2}\int \vec{E}(\vec{r}')\cdot\overleftrightarrow{G}(\vec{r}', \vec{r}_{\gtrless}) \times\{\epsilon(\omega)[\eta(z' + hf) - \eta(z')] + \eta(-z' - hf) - \eta(-z')\}\, d^3r' \tag{31}$$

used by Maradudin and Mills[3] which differs from the integral equation (15) in the sense that step functions appear in a different manner. Maradudin and Mills approximation

$$\epsilon[\eta(z' + hf) - \eta(z')] + \eta(-z' - hf) - \eta(-z') \approx (\epsilon - 1)hf\tfrac{1}{2}[\delta(z^+) + \delta 1(z^-)] \tag{32}$$

leads, instead of (25), to

$$\vec{\mathcal{E}}_T^{(1)}(\vec{\kappa}) = \pi F(\vec{\kappa} - \vec{\kappa}^{(0)})(\epsilon - 1)k_0^2[\vec{\mathcal{E}}_{T\parallel}^{(0)}\cdot\overleftrightarrow{G}(-\vec{\kappa}) + \tfrac{1}{2}(1 + \epsilon^2)\mathcal{E}_{Tz}^{(0)}\hat{z}\cdot\overleftrightarrow{G}(-\vec{\kappa})] . \tag{33}$$

Thus their results could be corrected by replacing $\frac{1}{2}(1+\epsilon^2)\mathcal{E}_{Tz}^{(0)}$ by $\epsilon\mathcal{E}_{Tz}^{(0)}$. Maradudin and Mills argued that since the zeroth-order fields are discontinuous, one should replace $\delta(z)$ in the expansion of step functions by $\frac{1}{2}[\delta(z^+) + \delta(z^-)]$. However we see that the derivation of the integral equation of the present paper automatically takes into account the discontinuous behavior of the fields and hence fixes uniquely the transmitted and scattered fields.[10]

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[7] The procedure we use in deriving the integral equation is similar to that used by E. Wolf [in *Coherence and Quantum Optics*, edited by L. Mandel and E. Wolf (Plenum, New York, 1973), p. 339] in the general formulation of integral equations, using the "vacuum" Green's function.

[8] The scattered fields do not contribute to the $\Sigma^{(\infty)}$ integral. This is because both the Green's function as well as the scattered fields satisfy the Sommerfeld radiation condition at infinity:

$$\lim_{r\to\infty} r[\vec{\nabla}\times\overleftrightarrow{G}(\vec{r}, \vec{r}') - ik_0\,\hat{r}\times\overleftrightarrow{G}(\vec{r}, \vec{r}')] = 0, \quad \hat{r} = \vec{r}/r$$

[cf. A. Sommerfeld, *Partial Differential Equations in Physics* (Academic, New York, 1949), p. 189; Chen-To Tai, *Dyadic Green's Function in Electromagnetic Theory* (Text Educational, San-Francisco, 1971)].

[9] These Green's function can be obtained from Eqs. (5.6), (5.23), and (5.43)–(5.46) of G. S. Agarwal, Phys. Rev. A 11, 230 (1975); and Eqs. (3.6) and (3.7) of G. S. Agarwal, *ibid.* 12, 1475 (1975); [noting that $G_{ij}(\vec{r}, \vec{r}') = k_0^{-2}\chi_{ijEE}(\vec{r}, \vec{r}', \omega)$], or from Appendix 'A' of Ref. 3.

[10] Juranek's prescription of surface currents has been incorporated in the Green's-function approach in a recent paper [D. L. Mills, Phys. Rev. B 12, 4036 (1975)].