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Optical properties of rough surfaces: General theory and the small roughness limit*

F. Toigo,† A. Marvin,‡ V. Celli, and N. R. Hill
Department of Physics, University of Virginia, Charlottesville, Virginia 22901
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The diffraction of electromagnetic waves from the rough surface of a material of finite permittivity is examined for the case where the wavelength of the incident radiation is comparable to the dimensions of the surface roughness. Two methods of calculation studied are the Rayleigh method and the extinction-theorem integral-equation method. The latter is shown to have a unique exact solution. This property is, in turn, used to show how the Rayleigh method can be modified to give convergent results. The extinction theorem is also used to reduce the Rayleigh equations to a simpler form. These reduced equations, which are extremely convenient to use in the case of small roughness, are applied in this case to find perturbative expressions for the reflected field and for the surface-plasmon dispersion relation.

I. INTRODUCTION

The general problem of the reflectivity of rough surfaces has attracted a great deal of interest in several separate connections: classical optics and the properties of diffraction gratings,[1] classical acoustics,[2] the interpretation of radar signals,[3] and, more recently, the study of the physical properties of well-characterized solid surfaces by atom scattering.[4,5] Because of the difference in background between people working in these areas, and because of the difference in emphasis on various aspects of the problem, the theory has been redeveloped fairly independently in each instance. The reflectivity formulas have been extensively examined in two limiting cases: the case of small roughness, when the height of the roughness is much smaller than the wavelength of the incident radiation,[6-9] and the case of large-scale roughness, when the surface profile varies slowly on the scale of the incident wavelength.[10,11] In the former case the appropriate form of perturbation theory can be applied, while in the latter one can use the semiclassical concepts of ray optics. However, there is still considerable uncertainty on how to construct a theory that is computationally convenient, that is exact in principle for the general case of arbitrary roughness, that reproduces the two extreme limits, and that shows how to obtain corrections in a systematic way.

The method originally proposed by Lord Rayleigh[2] in connection with problems of acoustics and later extended by Fano[1] to optical gratings leads to a divergent expression, if the surface profile is not sufficiently smooth.[12] A general explicit criterion for the validity of the original Rayleigh theory is still missing, but it is known that for a sinusoidal hard wall of equation $z = \zeta_0 \cos(2\pi x/a)$ the ratio ζ_0/a must be less than 0.072.[13-15]

However, it is possible to modify Rayleigh's procedure[16] in such a way that, at least in principle, convergence can always be achieved.[17,18] The necessary modifications are easily made for the case of the perfect conductor,[19] but become cumbersome when applied to a medium of finite permittivity and to our knowledge have never been presented explicitly. On the other hand, numerical calculations have shown that the original Rayleigh-Fano method does not always converge even for a medium of finite permittivity.[20]

Another method is based on obtaining integral equations that involve only the fields at the surface and their derivatives. This can be accomplished by using either the Lippmann-Schwinger equation[21,22] or, more simply and equivalently, Green's theorem[23-27] (i.e., Huygens' principle). When the integrals appearing in these methods are continued across the surface, one obtains a simple derivation of the classical extinction theorems of optics[28] (which can also be viewed as an "extended boundary condition" in the case of reflection from a perfect conductor). This crucial step, which has been taken more or less independently by several authors[22,23,25] leads directly to equations that are similar in form to the Rayleigh equations and equally convenient for computational purposes, but valid in principle without restriction. (The same equations have been obtained by DeSanto[29] by a somewhat different but equivalent procedure.)

It is the purpose of this paper to establish explicitly the relation between the Rayleigh and extinction-theorem methods for the general case of reflection at the surface of a medium of permittivity ϵ.[30] In the process we obtain a set of "reduced Rayleigh equations" that are extremely convenient for the discussion of the limit of small roughness.

We are especially interested in the application of the theory to the scattering of light from metal surfaces and the excitation of surface plasmons. The mathematical difficulties mentioned above are encountered in the theory of the reflection of scalar waves at rough surfaces as well as in the theory of electromagnetic waves. In addition, the vector nature of the electromagnetic field introduces a polarization dependence that is of considerable interest in itself. In particular, the incident light can couple resonantly to surface modes of the electromagnetic field (surface plasmons) and to surface phonons. The dispersion relation of these surface modes or surface excitations is itself affected by the roughness of the surface.[6,7,31]

We shall consider in detail a geometry of incidence where the field equations reduce to a single scalar equation, but the boundary conditions are such that the light can couple to surface modes. We can then study the full range of phenomena associated with the propagation of vector waves, such as the electromagnetic field, while retaining the simplicity of a scalar theory. Quite generally, of course, the reduction to independent scalar equations is always a desirable first step in the treatment of a vector problem.

In Sec. II we give a critical review of the Rayleigh-Fano (RF) theory, which will be cast in a form that facilitates comparison with the exact theory and also greatly simplifies the solution of the RF equations in the limit of small roughness. In Sec. III we develop the exact theory in a form that has great similarity to the RF method but is free from its limitations. In Sec. IV the relation between the two methods is fully explored. In Sec. V the theory is applied to find the reflectivity and the surface-plasmon dispersion relation in the limit of small roughness.

II. RAYLEIGH-FANO THEORY

We shall consider a P-polarized wave incident on a medium of dielectric constant ϵ bounded by the surface of equation $z=\zeta(y)$ that lies generally parallel to the plane $z=0$. The medium occupies the half space $z>\zeta$, the frequency of the incoming radiation is ω, the plane of incidence is the plane $x=0$. Since we assume that the surface is smooth in the x direction, all reflected waves also lie in the plane $x=0$, with an electric field vector in that plane and a magnetic field pointing in the x direction. Let $B(y,z)$ be the x component of the magnetic field and let superscripts "out" and "in" denote the field outside and inside the medium. B obeys a scalar wave equation and suffices, with appropriate boundary conditions, to give a full description of the scattering.

The continuity conditions at the surface $z=\zeta(y)$ are

$$B^{\rm in}(y,\zeta(y))=B^{\rm out}(y,\zeta(y)), \tag{2.1a}$$

$$\frac{1}{\epsilon}\frac{\partial B^{\rm in}}{\partial n}=\frac{\partial B^{\rm out}}{\partial n}, \tag{2.1b}$$

with

$$\frac{\partial}{\partial n}=[1+\zeta'(y)^2]^{-1/2}\left(\frac{\partial}{\partial z}-\zeta'(y)\frac{\partial}{\partial y}\right). \tag{2.2}$$

For most applications we suppose that $\zeta(y)$ is a periodic function of period a, so that we can write

$$\zeta(y)=\sum_n \zeta_n e^{iG_n y}, \tag{2.3}$$

with $G_n=2\pi n/a$. However, much of the following development still holds for a general $\zeta(y)$, provided only that the discrete sum in (2.3) is replaced by a Fourier integral. Alternatively, we can simply take the limit $a\to\infty$ in the formulas for a periodic surface, with the understanding that $\sum_k \to a\int dK/2\pi$. If the incident wave vector has components K_0 and p_0 parallel and perpendicular to the surface, with $K_0^2+p_0^2=\omega^2/c^2$, the incident field is

$$B_i e^{i(K_0 y+p_0 z)}, \tag{2.4}$$

and the reflected field for $z\to-\infty$ is

$$\sum_n B_n e^{i(K_n y-p_n z)}, \tag{2.5}$$

with $K_n=K_0+G_n$ and

$$K_n^2+p_n^2=\omega^2/c^2. \tag{2.6}$$

Similarly for $z\to+\infty$, the refracted field is

$$\sum_n C_n e^{i(K_n y+q_n z)}, \tag{2.7}$$

with

$$K_n^2+q_n^2=\epsilon\omega^2/c^2. \tag{2.8}$$

For a nonperiodic surface we shall use a quasicontinuous variable $K'=K_0+G$ instead of K_n. Then (2.5) and (2.7) become, respectively,

$$\sum_{K'} B(K')e^{i(K'y-p'z)}, \tag{2.5$'$}$$

$$\sum_{K'} C(K')e^{i(K'y+q'z)}, \tag{2.7$'$}$$

with

$$K'^2+p'^2=\omega^2/c^2, \tag{2.6$'$}$$

$$K'^2+q'^2=\epsilon\omega^2/c^2. \tag{2.8$'$}$$

If we assume that the expressions (2.5′) and (2.7′) can be continued up to the surface $z=\zeta(y)$ and impose the condition (2.1), we find

$$\sum_{K'} [-e^{-ip'\zeta(y)} e^{iK'y} B(K') + e^{iq'\zeta(y)} e^{iK'y} C(K')] = B_i e^{ip_0\zeta(y)} e^{iK_0 y}, \tag{2.9a}$$

$$\sum_{K'} \left([p'+K'\zeta'(y)] e^{-ip'\zeta(y)} e^{iK'y} B(K') + \frac{1}{\epsilon}[q'-K'\zeta'(y)] e^{iq'\zeta(y)} e^{iK'y} C(K')\right) = [p_0 - K_0\zeta'(y)] B_i e^{ip_0\zeta(y)} e^{iK_0 y}, \tag{2.9b}$$

where the sum over K' reduces to a sum over $K_n = K_0 + G_n$ for a periodic surface. By taking Fourier transforms of both sides, with the definition

$$(e^{ip'\zeta})_{K-K'} = \int_0^a e^{ip'\zeta(y)} e^{-i(K-K')y} \frac{dy}{a}, \tag{2.10}$$

we obtain after some manipulation the RF equations[1,19,31]

$$\sum_{K'} [-(e^{-ip'\zeta})_{K-K'} B(K') + (e^{iq'\zeta})_{K-K'} C(K')] = B_i (e^{ip_0\zeta})_{K-K_0}, \tag{2.11a}$$

$$\sum_{K'} \frac{(\omega/c)^2 - KK'}{p'} (e^{-ip'\zeta})_{K-K'} B(K') + \frac{\epsilon(\omega/c)^2 - KK'}{\epsilon q'} (e^{iq'\zeta})_{K-K'} C(K') = B_i \frac{(\omega/c)^2 - KK_0}{p_0} (e^{ip_0\zeta})_{K-K_0}. \tag{2.11b}$$

We remark that these are coupled equations for B and C and that the matrix elements of the kernel, of the type $(e^{-ip'\zeta})_{K-K'}$ are not symmetric functions of K and K', since $p = [(\omega/c)^2 - K^2]^{1/2}$ does not appear in the exponent.

It is possible to obtain a separate equation for C and at the same time to obtain a more symmetric kernel by multiplying (2.9a) and (2.9b), respectively, by the factors $[p - K\zeta'(y)]\exp[-ip\zeta(y) - iKy]$ and $\exp[-ip\zeta(y) - iKy]$, summing side by side and integrating over y. We find, using the identities given in Appendix A,

$$(\epsilon - 1)\sum_{K'} \frac{KK' + pq'}{q' - p} (e^{i(q'-p)\zeta})_{K-K'} C(K') = 2\epsilon p_0 B_i \delta_{K,K_0}. \tag{2.12}$$

Essentially the same equation has been obtained by Waterman[25] starting from the extinction theorem. We will return to this point in Sec. V. By a similar procedure, using the factors $[q + K\zeta'(y)]\exp[iq\zeta(y) - iKy]$ and $-\epsilon \times \exp[iq\zeta(y) - iky]$, we find a separate equation for the reflected amplitude B:

$$\sum_{K'} \frac{KK' + qp'}{q - p'} (e^{i(q-p')\zeta})_{K-K'} B(K') = -\frac{KK_0 - qp_0}{q + p_0} (e^{i(q+p_0)\zeta})_{K-K_0} B_i. \tag{2.13}$$

We can also multiply Eq. (2.9) by factors containing $\exp[ip\zeta(y)]$, instead of $\exp[-ip\zeta(y)]$, and proceed as above. We obtain then instead of (2.12)

$$2\epsilon p B(K) = (1-\epsilon)\sum_{K'} \frac{KK' - pq'}{p + q'} (e^{i(p+q')\zeta})_{K-K'} C(K'), \tag{2.14}$$

and, similarly, instead of (2.13),

$$2qC(K) = (1-\epsilon)\left(\frac{KK_0 + p_0 q}{p_0 - q} (e^{i(p_0-q)\zeta})_{K-K_0} B_i - \sum_{K'} \frac{KK' - qp'}{q + p'} (e^{-i(q+p')\zeta})_{K-K'} B(K')\right). \tag{2.15}$$

This is as close as we can come to an explicit solution of the Rayleigh-Fano equations. The physical meaning of the transformations leading to (2.12)–(2.15) is discussed in Sec. III in connection with the extinction theorem.

III. INTEGRAL EQUATIONS AND EXTINCTION THEOREMS

It is well known how Maxwell's differential equations can be converted into integral equations.[32] In the case under consideration, we introduce the outgoing-wave Green's function of free space:

$$G_0(r) = r^{-1} e^{ik_0 r}, \tag{3.1}$$

with $k_0 = \omega/c$, and the Green's function of a medium of dielectric constant ϵ

$$G(r) = r^{-1} e^{ik_\epsilon r}, \tag{3.2}$$

with $k_\epsilon = \epsilon^{1/2}\omega/c$. For $\epsilon < 0$, $k_\epsilon = i|\epsilon|^{1/2}\omega/c$. Application of Green's theorem (Huygens' principle) to the empty half space below the surface of the medium gives

$$B_i(\vec{r}) - \frac{1}{4\pi}\int d\vec{S}' \cdot [B^{\text{out}}(\vec{r}')\vec{\nabla}' G_0(|\vec{r} - \vec{r}'|) - G_0(|\vec{r} - \vec{r}'|)\vec{\nabla}' B^{\text{out}}(\vec{r}')] = \begin{cases} B^{\text{out}}(\vec{r}) & \text{for } z < \zeta(y), \\ 0 & \text{for } z > \zeta(y), \end{cases} \tag{3.3}$$

where the integral is taken over the surface $z'=\zeta(y')$. We introduce the field on the surface and its normal derivative on the vacuum side

$$H(y')=B^{\text{out}}(0,y',\zeta(y')), \tag{3.4}$$

$$L(y')=[1+\zeta'^2(y')]^{1/2}\left(\frac{\partial B^{\text{out}}(0,y',z')}{\partial n'}\right)_{z'=\zeta(y')}, \tag{3.5}$$

and stipulate that G_0 and its normal derivative must be evaluated for $z'=\zeta(y')$. Using (2.2), (3.3) can be rewritten, for incidence in the plane $x=0$,

$$B_i-\frac{1}{4\pi}\int dx'\,dy'\left[H\left(\frac{\partial G_0}{\partial z'}-\zeta'\,\frac{\partial G_0}{\partial y'}\right)-G_0L\right]=\begin{cases}B^{\text{out}} & \text{for } z<\zeta(y), \quad (3.6\text{a})\\ 0 & \text{for } z>\zeta(y), \quad (3.6\text{b})\end{cases}$$

where all functions are evaluated at $x=0$ [thus $B_i\equiv B_i(0,y,z)$, etc.]. Equation (3.6b) expresses the extinction theorem[23,28,32]: the field and its derivative on the surface act as sources that "extinguish" the incoming field in the medium.

Two equations of the same type are obtained by applying Green's theorem to the half space occupied by the medium. Taking into account the continuity conditions (2.1) we have

$$\frac{1}{4\pi}\int dx'\,dy'\left[H\left(\frac{\partial G}{\partial z'}-\zeta'\,\frac{\partial G}{\partial y'}\right)-\epsilon GL\right]=\begin{cases}0 & \text{for } z<\zeta(y), \quad (3.7\text{a})\\ B^{\text{in}} & \text{for } z>\zeta(y). \quad (3.7\text{b})\end{cases}$$

Here again Eq. (3.7a) expresses the extinction theorem. Equations (3.6) and (3.7) are not mutually independent. A complete set of equations that is sufficient to determine the field on the surface and its derivative is obtained by letting $z\to\zeta(y)$ in (3.6a) from below and (3.7b) from above, so that the right-hand side of both equations is $H(y)$. Alternatively, one can take the limit $z\to\zeta(y)$ from above in (3.6b) and from below in (3.7a). The compatibility of these possible procedures follows from the fact that the normal derivatives $\partial G_0/\partial n'$ and $\partial G/\partial n'$ computed for $z'=\zeta(y')$, have a discontinuity $4\pi\delta(x-x')\times\delta(y-y')$ in going from above to below the surface $z=\zeta(y)$.

Once the self-consistent equations on the surface have been solved for H and L, the diffracted and refracted fields can be found from (3.6) for $z\to-\infty$ and (3.7) for $z\to+\infty$, respectively. Explicit formulas are obtained by Fourier transforming H, L, B^{out}, and B^{in} and using the integral representations

$$G_0(\vec{r}-\vec{r}')=\frac{i}{2\pi}\int d^2K\,\frac{e^{ip|z-z'|}}{p}\,p^{i\vec{K}\cdot(\vec{R}-\vec{R}')}, \tag{3.8}$$

$$G(\vec{r}-\vec{r}')=\frac{i}{2\pi}\int d^2K\,\frac{e^{iq|z-z'|}}{q}\,e^{i\vec{K}\cdot(\vec{R}-\vec{R}')}, \tag{3.9}$$

where $\vec{R}=(x,y,0)$, $p^2+K^2=\omega^2/c^2$, and $q^2+K^2=\epsilon\omega^2/c^2$. To find the reflection coefficients B^{out} must be evaluated for $z\to-\infty$; then $|z-z'|$ in (3.8) can be replaced by $z'-z$, with the result that

$$B^{\text{out}}(K,z)=B_i\delta_{KK_0}e^{ip_0z}+\frac{1}{2}\sum_{K'}\frac{e^{-ip\zeta}}{p^2}(e^{ip\zeta})_{K-K'}\times\left\{\left[\left(\frac{\omega}{c}\right)^2-KK'\right]H(K')+ipL(K')\right\}. \tag{3.10}$$

The heart of the problem however lies in finding H and L. The self-consistent equations discussed above are rather unmanageable in general, because both the source points and the observation points lie on the surface $z=\zeta(y)$.

More manageable equations are obtained if the observation points are taken on planes $z=\text{const}$ that lie outside the selvedge region, i.e., for $z<\min\zeta(y)$ or $z>\max\zeta(y)$. The essential simplification arises from the fact that $z-z'$ in (3.8) and (3.9) does not change sign, and therefore it is not necessary to take the absolute value. Using the extinction-theorem equations (3.6b) and (3.7a) and the Fourier representations (3.8) and (3.9) one obtains convenient equations for H and L:

$$a^{-1}\int dy\{[p-K\zeta'(y)]H(y)-iL(y)\}\times e^{-iKy-ip\zeta(y)}=2pB_i\delta_{KK_0}, \tag{3.11}$$

$$a^{-1}\int dy\{i[q+K\zeta'(y)]H(y)-\epsilon L(y)\}\times e^{-iKy+iq\zeta(y)}=0. \tag{3.12}$$

It is clear by construction that the correct boundary values of the field and its normal derivative, H and L, satisfy the extinction-theorem equations (3.11) and (3.12). It can also be shown that these equations are sufficient to determine H and L uniquely, or in other words that the corresponding homogeneous equations (with $B_i = 0$) have only the trivial solution $H = 0$, $L = 0$, except for the particular frequencies where undamped surface plasmons occur. The proof is as follows: the left-hand sides of (3.6) and (3.7), for any square-integrable $H(y')$ and $L(y')$, represent functions of y and z that are analytic in each of these variables and are solutions of the Helmholtz equation except for $z = \zeta(y)$. Now every solution H, L of (3.11) and (3.12) satisfies the extinction theorem (3.6b) for all $z > \zeta(y)$ and (3.7a) for all $z < \zeta(y)$ by the principle of analytic continuation, even though (3.11) and (3.12) were established by using the extinction theorems outside the selvedge region. Then (3.6a) and (3.7b) give the fields everywhere with the correct matching conditions and represent the unique solution of the Helmholtz equation. Thus H and L must be uniquely determined by (3.11) and (3.12) up to functions of measure zero that would not change the value of the left-hand sides of (3.6) and (3.7).

The solution of (3.11) and (3.12) can only be obtained numerically by some sequence of successive approximations. One convenient procedure is to expand H in Fourier series

$$H(y) = \sum_{K'} e^{iK'y} H(K')$$

and similarly for $L(y)$. Using identities such as $-ip\zeta' e^{-ip\zeta} = de^{-ip\zeta}/dy$ and integrations by parts, the resulting equations can be written

$$\sum_{K'} \left(\frac{(\omega/c)^2 - KK'}{p} H(K') - iL(K') \right) \times (e^{-ip\zeta})_{K-K'} = 2pB_i \delta_{KK_0}, \quad (3.11')$$

$$\sum_{K'} \left(\frac{\epsilon(\omega/c)^2 - KK'}{\epsilon q} H(K') + iL(K') \right) \times (e^{iq\zeta})_{K-K'} = 0. \quad (3.12')$$

For a periodic surface, the sum over K' reduces to a sum over $K_{n'} = K_0 + G_{n'}$ in the usual way. One can then keep only $2N$ equations for N values of K_n and solve for the first $2N$ coefficients $H_n \equiv H(K_n)$ and $L_n \equiv L(K_n)$.

IV. RELATION BETWEEN THE RAYLEIGH METHOD AND EXTINCTION THEOREM

The set of Rayleigh equations (2.11) is a matrix equation for $B(K)$ and $C(K)$; the set of extinction equations (3.11′) and (3.12′) is a matrix equation for $H(K)$ and $L(K)$. It is apparent that these matrices have similar elements. Specifically, when the surface profile is symmetric they become the transposes of each other (see Appendix B). We expect then that the uniqueness of the solution to the extinction equations has important consequences for the Rayleigh method. The mathematical arguments put forth by Millar[18] receive a physical interpretation in this light and are easily extended to a medium of finite permittivity.

Let us look at (3.11) for the case of a perfect conductor and a periodic surface with the boundary condition $L(y) = 0$ for P polarization and normal incidence. We get

$$\frac{1}{a} \int_0^a dy \, [p_n - G_n \zeta'(y)] \times e^{-iG_n y - ip_n \zeta(y)} H(y) = 2p_0 B_i \delta_{n0} \quad (4.1)$$

for all n. Since the solution to these equations is unique, it must be true that the set of functions $\beta_n(y) = [p_n - G_n \zeta'(y)] e^{-iG_n y - ip_n \zeta(y)}$ is complete. Let us also look at the Rayleigh equation for the same case. It is

$$\sum_n [p_n - G_n \zeta'(y)] e^{-iG_n y - ip_n \zeta(y)} B(-K_n) = p_0 B_i e^{+ip_0 \zeta(y)}, \quad (4.2)$$

which is an attempt to expand the function on the right-hand side in terms of the basis $\beta_n(y)$. Since the set $\beta_n(y)$ is complete, given any η_1, we can find N_1 large enough that some combination of the first N_1 function $\beta_n(y)$ will approximate the right-hand side to a mean-square difference less than η_1. But, since the $\beta_n(y)$ are not orthogonal, when we take some $\eta_2 < \eta_1$, requiring $N_2 \geq N_1$ terms, all of the coefficients $B(K_n)$ may change including those for $n < N_1$; that is, for a oblique basis, there is no finality of coefficients.[33] For this reason the expansion may diverge. This, of course, can be remedied by using a new basis set of functions which consist of some linear combinations of the $\beta_n(y)$. In particular, a basis set resulting from the orthogonalization of the $\beta_n(y)$ will always give convergent series.[34] This argument can be generalized to cases of non-normal incidence by comparing the extinction equations for an incidence angle of θ with the Rayleigh equation for an angle $-\theta$, as done in Appendix C.

By examining the extinction equation and the Rayleigh method for a perfect conductor and S-polarized light one finds instead of (4.1) and (4.2)

$$\frac{1}{a} \int_0^a dy \, e^{-iG_n y - ip_n \zeta(y)} L(y) = 2p_0 E_i \delta_{n0}, \quad (4.1')$$

$$\sum_n e^{-iG_n y - ip_n \zeta(y)} E(-K_n) = E_i e^{ip_0 \zeta(y)}, \quad (4.2')$$

where E is the x component of the electric field and L its normal derivative at the surface. (The boundary condition now is that E vanishes at the surface.) Proceeding as before, we see that the set $\alpha_n(y)=e^{-ip_n\zeta(y)}e^{-iK_ny}$ appearing in (2.9) is also complete. Further, by repeating these two cases, but with the vacuum replaced by a medium of permittivity ϵ, we can show that the remaining two sets of functions in (2.9) are complete. It can then be concluded that the Rayleigh equations (2.9) are valid but that solutions by simple developments such as (2.11) may diverge. This can be corrected by properly choosing a new set of functions consisting of combinations of the original ones. Orthogonalization is one combination that always results in a set with which there will be convergence, but it, and to a somewhat lesser extent, equivalent variational methods are complicated in the case of a medium of finite permittivity.

It is possible to show directly that the Rayleigh solution satisfies the extinction equations (3.11) and (3.12). Explicitly, the Rayleigh expression for the refracted field (2.7′), gives

$$H(y)=\sum_{K'} C(K')e^{iq'\zeta(y)+iK'y}, \tag{4.3}$$

$$\epsilon L(y)=i\sum_{K'}[q'-K'\zeta'(y)]C(K')e^{iq'\zeta(y)+iK'y}. \tag{4.4}$$

These expressions satisfy (3.12) identically and give the "reduced" Rayleigh equation (2.12) for $C(K)$ when substituted in (3.11). To show this one uses certain "orthonormality relations" that are listed in Appendix A. Similarly, the Rayleigh expression for the reflected field [Eq. (2.5′)], gives

$$H(y)=B_ie^{ip_0\zeta(y)+iK_0y}+\sum_{K'}B(K')e^{-ip'\zeta(y)+iK'y}, \tag{4.5}$$

$$L(y)=iB_i[p_0-K_0\zeta'(y)]e^{ip_0\zeta(y)+iK_0y} -i\sum_{K'}B(K'[p'+K'\zeta(y)]e^{-ip'\zeta(y)+iK'y}. \tag{4.6}$$

Now we find that (3.11) is identically satisfied and that (3.12) gives the "reduced" Rayleigh equation (2.13). Again we make use of the relations listed in Appendix A.

Finally, we wish to use the extinction theorem to show the physical meaning of the tranformations which were used to obtain (2.12) and (2.13). The sum

$$\sum_{K'} e^{iq'\zeta(y)}e^{iK'y}C(K')$$

appearing in (2.9a) is equal to the field along the surface, $H(y)$; likewise, in (2.9b) the sum containing the $C(K')$ is equal to $L(y)$. If we multiply the former by $[1+\zeta'^2(y)]^{1/2}\partial G_0/\partial n'$ and the latter by G_0, Eq. (3.6b) tells us that the integral of the difference will be equal to zero when $z>\zeta(y)$. The steps used to obtain (2.13), in which $C(K)$ has been eliminated, are an implementation of the above procedure for $z>\max[\zeta(y)]$. This becomes very apparent if the above Green's-function integral is reduced using (3.8) for $z>\max[\zeta(y)]$.

V. SMALL-ROUGHNESS LIMIT

In this section we show how simply one can obtain the reflection coefficient and the dispersion relation for surface plasmons from the reduced Rayleigh equations of Sec. II. The results have been obtained previously by much more cumbersome versions of perturbation theory.[6,8,9] With the present method it is easy, if desired, to obtain higher-order corrections.

For small roughness we can solve (2.13) by iteration, putting

$$(e^{i(q-p')\zeta})_{K-K'}=\delta_{KK'}+i(q-p')\zeta_{K-K'}+\cdots. \tag{5.1}$$

To lowest order we find the specularly reflected amplitude, which can be written

$$B(K)=\delta_{KK_0}B_i\frac{\epsilon p_0-q_0}{\epsilon p_0+q_0}, \tag{5.2}$$

by use of the identities

$$q^2-p^2=(\epsilon-1)(\omega/c)^2, \tag{5.3a}$$

$$(K^2+pq)(p+q)=(\epsilon p+q)(\omega/c)^2, \tag{5.3b}$$

$$(K^2-pq)(p-q)=(\epsilon p-q)(\omega/c)^2. \tag{5.4}$$

By inserting (5.2) back into (2.13) we find the lowest-order result for the diffusely reflected field (for $K\neq K_0$):

$$B(K)=2iB_i(1-\epsilon)p_0\zeta_{K-K_0}\frac{\epsilon KK_0-qq_0}{(\epsilon p+q)(\epsilon p_0+q_0)}. \tag{5.5}$$

In a similar way, we can find the surface-plasmon dispersion relation by putting $B_i=0$ and requiring that the resulting homogeneous equations have a nonzero solution. For a flat surface the dispersion relation is given by $\epsilon p+q=0$, corresponding to the vanishing of the denominator in (5.2). Recalling that p and q are pure imaginary for real negative ϵ, we put $p=i\beta$, $q=i\gamma$, with

$$\beta=[K^2-(\omega/c)^2]^{1/2},\quad \gamma=[K^2-\epsilon(\omega/c)^2]^{1/2}. \tag{5.6}$$

By use of the identity (5.3b) the dispersion relation $\epsilon\beta+\gamma=0$, can also be written $K^2-\beta\gamma=0$, and from these two expressions it also follows that $K^2+\gamma^2/\epsilon=0$ or $K^2+\epsilon\beta^2=0$, or more explicitly $(\epsilon+1)K^2=\epsilon(\omega/c)^2$. The dispersion relation for a rough surface can be written in an even greater variety of equivalent ways. To second order in ζ, we find from (2.13) (with $B_i=0$) and (5.1)[31]

$$\epsilon\beta+\gamma=\sum_{K'}|\zeta_{K-K'}|^2(1-\epsilon)^2\frac{(KK'-\beta\gamma')(KK'-\beta'\gamma)}{\epsilon\beta'+\gamma'}. \tag{5.7}$$

This equation, when solved for ω as a function of K, gives both the dispersion relation and the lifetime of the surface plasmon, from the real and imaginary parts of $\omega(K)=\omega_R(K)+i\Gamma(K)$. A contribution to Γ arises from two sources: the imaginary part of ϵ, corresponding to electron-hole excitations or interband transitions, and the fact that β' is imaginary (i.e., p' is real) for $K'<\omega/c$, giving a complex denominator $-i\epsilon p'+\gamma'$ on the right-hand side of (5.7). The latter contribution is clearly due to the radiative decay of the surface plasmon in the presence of surface roughness. In the case of a periodic surface profile, as in a grating, the sum over K' involves only the values $K_n=K+G_n$, as discussed in Sec. II. When $K=-\frac{1}{2}G_n$ for some n (i.e., the condition for Bragg diffraction of the surface plasmon is satisfied), the denominator on the right-hand side of (5.7) vanishes and a gap opens in the $\omega(K)$ curve. By keeping only the nth term in the sum we find that the frequencies on the two sides of the gap are given by the solutions of

$$\epsilon\beta+\gamma=\pm|\zeta_n|(1-\epsilon)(K^2+\beta\gamma), \tag{5.8}$$

with $K=-\pi n/a$. The factor $(K^2+\beta\gamma)$ on the right-hand side can also be written $2K^2$ or $2\beta\gamma$, since $K^2=\beta\gamma$ to lowest order.

The scattered field (5.5) exhibits a resonance when the surface-plasmon condition $\epsilon p+q=0$ is satisfied. For a grating, a marked resonant behavior (Wood's anomaly) will be obtained in the specular and diffracted intensities.

The perturbation expansion we have employed above can be continued formally to arbitrary order in ζ. If the expansion converges, it appears that the Rayleigh-Fano equations have a unique solution, which in the limit $\zeta=0$ is the correct solution of the scattering problem. The range of convergence of this expansion in powers of ζ depends on the shape of the function $\zeta(x)$ and is presumably the same as the range of validity of the Rayleigh method itself.

The generalization of these results to a random surface is not difficult, since each Fourier component of the surface roughness, $\zeta_{\vec{K}-\vec{K}'}$, contributes separately to the final formulas and can thus be treated independently. The formulas for the reflection coefficients have been obtained by other methods and are well established.[7,8] The formulas for the surface-plasmon dispersion can be simply obtained from (5.7) by allowing $\vec{K}$ and $\vec{K}'$ to be two-dimensional vectors and replacing KK' by $\vec{K}\cdot\vec{K}'$. This formula is equivalent to those obtained by Maradudin and Zierau[9] by a method that is not devoid of ambiguities.

VI. CONCLUSIONS

We have investigated in detail the relation between the Rayleigh method for the solution of the problem of scattering from a rough surface and the extinction theorem of optics. Since the extinction theorem is valid without restriction, one can deduce from this relation that the set of functions employed in the Rayleigh method are complete, although the Rayleigh expansion itself need not converge. Many different versions of the theory can be obtained by using these sets of functions to carry out projections and expansions. By this technique, we have been able to show explicitly that the Rayleigh method and the extinction theorem are in a sense equivalent. It should be noted however that the projection procedure [as in going from (2.9) to (2.12)] is always valid, while the expansion procedure [as in going from (3.11) to (2.12) by (4.3) and (4.4)] suffers the same limitations as the original Rayleigh method, i.e., it does not converge in general unless it is preceded by an appropriate rearrangement, such as orthogonalization of the basis sets.

We have considered several possible systems of equations and have found that the "reduced Rayleigh equation" (2.13) is most convenient for the treatment of the small-roughness limit. We have given an illustration of this by showing how the surface-plasmon dispersion relation on a rough surface can be found in a simple and unambiguous manner.

We have also carried out some numerical calculations in the case of finite roughness, which will be reported separately, along with a discussion of the theory in the semiclassical limit. Here we remark only that the reduced equation (2.13) is not convenient for such calculations in the case of large negative ϵ (reflection from metals). It is easier to use the original Rayleigh equations in their range of validity or the extinction theorem, partly because then the factors of the type $\exp[ip\zeta(y)]$ involve only real or imaginary exponents.

Finally we note that the shape of the surface profile $\zeta(y)$ need not be given by an analytic function for the extinction theorem to be valid or for the small-roughness expansion to hold. To make sure of this, we have solved the self-consistent equations of Huygens' principle, (3.6a) and (3.7b), for a saw-tooth profile by consistently keeping only the lowest-order terms in the height of the saw tooth. After lengthy manipulations, the results can be shown to be equivalent to those reported in Sec. V, with the appropriate $\zeta_{K-K'}$.

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APPENDIX A

We list here a number of relations that prove useful in showing the equivalence of various formulations of the scattering problem for a corrugated surface:

$$\int dy\,[p-p'+(K+K')\zeta'(y)] \times e^{i(p+p')\zeta(y)}e^{-i(K-K')y}=0, \quad \text{(A1)}$$

$$\int dy\,[q-q'+(K+K')\zeta'(y)] \times e^{i(q+q')\zeta(y)}e^{-i(K-K')y}=0, \quad \text{(A1')}$$

$$\int dy\,[p+p'+(K+K')\zeta'(y)] \times e^{i(p-p')\zeta(y)}e^{-i(K-K')y}=2pa\delta_{KK'}, \quad \text{(A2)}$$

$$\int dy\,[q+q'+(K+K')\zeta'(y)] \times e^{i(q-q')\zeta(y)}e^{-i(K-K')y}=2qa\delta_{KK'}. \quad \text{(A2')}$$

To prove (A1), integrate by parts using

$$\zeta' e^{i(p+p')\zeta}=\frac{1}{i(p+p')}\frac{d}{dz}e^{i(p+p')\zeta}, \quad \text{(A3)}$$

and note that $p^2-p'^2=-(K^2-K'^2)$. To prove (A2) proceed in the same way, except that $p'\to -p'$ and the term with $K=K'$ (and $p=p'$) has to be treated separately. To obtain (A1') and (A2'), simply let $p\to q$. Additional relations of a similar type are obtained by taking the complex conjugate and also by changing the sign of K and K'.

APPENDIX B

We show here explicitly the formal relation between the Rayleigh kernel and the extinction-theorem kernel. The Rayleigh-Fano equations (2.11) can be written $\sum_{K'} \underline{M}_{KK'}\underline{B}_{K'}=\underline{R}_K B_i$, where, setting $k_0=\omega/c$,

$$\underline{M}_{KK'}=\begin{pmatrix} -(e^{-ip'\zeta})_{K-K'} & (e^{iq'\zeta})_{K-K'} \\ [(k_0^2-KK')/p'](e^{-ip'\zeta})_{K-K'} & [(\epsilon k_0^2-KK')/\epsilon q'](e^{iq'\zeta})_{K-K'} \end{pmatrix},$$

$$\underline{B}_{K'}=\begin{pmatrix} B(K') \\ C(K') \end{pmatrix}, \quad \underline{R}_K=\begin{pmatrix} (e^{ip_0\zeta})_{K-K_0} \\ [(k_0^2-KK_0)/p_0](e^{ip_0\zeta})_{K-K_0} \end{pmatrix}.$$

In a similar notation, the extinction-theorem equations (3.11') and (3.12') are written $\sum_{K'}\underline{\tilde{M}}_{KK'}\underline{H}_{K'}=\underline{E}_K B_i$, where

$$\underline{\tilde{M}}_{KK'}=\begin{pmatrix} -(e^{-ip\zeta})_{K-K'} & [(k_0^2-KK')/p](e^{-ip\zeta})_{K-K'} \\ (e^{iq\zeta})_{K-K'} & [(\epsilon k_0^2-KK')/\epsilon q](e^{iq\zeta})_{K-K'} \end{pmatrix},$$

$$\underline{H}_{K'}=\begin{pmatrix} iL(K') \\ H(K') \end{pmatrix}, \quad \underline{E}_K=2p\delta_{K,K_0}\begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

If the surface profile is symmetric, i.e., if $\zeta(-y)=\zeta(y)$, one sees that $\underline{\tilde{M}}_{K'K}$ is the transpose of $\underline{M}_{KK'}$. Then the kernel of the Rayleigh-Fano method is the transpose of the kernel of the extinction method.

APPENDIX C

The extinction equation (3.11) for the case of a perfect conductor and a periodic surface and for light of p polarization and incidence angle θ is

$$\frac{1}{a}\int_0^a dy\,[p_n-K_n\zeta'(y)]e^{-iK_ny-ip_n\zeta(y)}H(y)=2p_0B_i\delta_{n0}, \quad \text{(C1)}$$

where $K_n=(\omega/c)\sin\theta+G_n$ and $p_n^2=(\omega/c)^2-K_n^2$. The Rayleigh equation for the same case and incidence angle θ_r is

$$\sum_n [p_n^r+K_n^r\zeta'(y)]e^{iK_n^ry-ip_n^r}B_n =[p_0^r-K_0^r\zeta'(y)]B_ie^{ip_0\zeta(y)}e^{iK_0y}. \quad \text{(C2)}$$

If we choose $\theta_r=-\theta$ we have $K_n=-K_{-n}^r$ and $p_n=p_{-n}^r$ so that (C1) is

$$\frac{1}{a}\int_0^a dy\,[p_{-n}^r+K_{-n}^r\zeta'(y)] \times e^{iK_{-n}^r-ip_{-n}^r\zeta(y)}H(y)=2p_0^rB_i\delta_{n,0}. \quad \text{(C3)}$$

The argument following (4.2) can now be applied to (C3) to show that the set of functions appearing in (C2) is complete.

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†Permanent address: Istituto di Fisica, Unità GNSM del CNR, via Marzolo 35100 Padua, Italy.

‡Permanent address: Istituto di Fisica Teorica, Università di Trieste, Trieste, Italy.

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[34]The same sort of situation arises in simple complex analysis. For example, while the powers $1, x, x^2, \ldots$ form a complete set, they cannot give a convergent series which represents say $(x+\frac{1}{2})^{-1}$ in the interval $0<x<1$ because of the pole at $x=-\frac{1}{2}$. However, $(x+\frac{1}{2})^{-1}$ can be expanded in the set 1, $(x-\frac{1}{2})$, $(x-\frac{1}{2})^2, \ldots$, giving the series $\sum_n (-1)^n (x-\frac{1}{2})^n$, which converges for $-\frac{1}{2}<x<\frac{3}{2}$. Moreover, any regular function can be expanded over the interval $(0,1)$ in the appropriate orthogonal set, the shifted Legendre polynomials $L_n(2x-1)$.