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# Surface plasmons on a large-amplitude grating

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Dispersion relations are obtained by two different methods for surface plasmons (in the nonretarded limit) propagating on the surface of a dielectric medium on which a large-amplitude grating has been ruled. The first method is based on the Rayleigh hypothesis; the second method is based on the extinction-theorem form of Green's theorem. It is found that there is an infinite number of branches of the surface-plasmon dispersion curve. Numerical solutions of the dispersion relations are obtained in the case that the dielectric medium is a free-electron metal for two surface profiles: a sinusoidal profile and a symmetric sawtooth profile. For the former profile, results are obtained for corrugation strengths far exceeding the value for which the Rayleigh hypothesis ceases to be valid.

## I. INTRODUCTION

Recent experimental[1,2] and theoretical[3,4] work on the propagation of surface plasmons[5] over a randomly rough, planar surface has shown that in the presence of surface roughness each branch of the surface-plasmon dispersion curve for a perfectly flat surface is split into two branches.

The theoretical work on this problem[3,4] has been carried out in the limit of small roughness. Because real surfaces can be rougher than those to which the small roughness limit is applicable, it is of interest to obtain the dispersion curve for surface plasmons on a very rough surface. Unfortunately, such a calculation appears to be very difficult at the present time if the surface is randomly rough.

The situation is quite different if the profile of the rough surface is deterministic and periodic. In this case it is possible to obtain a dispersion relation for surface plasmons that is formally exact, irrespective of the strength of the roughness. In this paper we present the derivation of such a dispersion relation, and numerical solutions of it, for two different surface profiles, in the expectation that the results will provide some insights into the nature of the corresponding dispersion curve for surface plasmons on a randomly rough surface.

We consider here a surface plasmon propagating perpendicularly to the grooves of a grating, whose profile is given by the equation $x_3=\zeta(x_1)$, where the surface profile function $\zeta(x_1)$, is a periodic function of $x_1$ with period $a$. The region defined by $x_3>\zeta(x_1)$ is a vacuum, while the region $x_3<\zeta(x_1)$ is filled by a dielectric medium characterized by an isotropic, frequency-dependent dielectric tensor $\epsilon_{\mu\nu}(\omega)=\delta_{\mu\nu}\,\epsilon(\omega)$. The region $\zeta_{\min}<x_3<\zeta_{\max}$ is called the selvedge region.

We seek the solution of Laplace's equation

$$\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_3^2}\right)\varphi(x_1x_3\,|\,\omega)=0\,, \tag{1.1}$$

for a $p$-polarized surface plasmon propagating in the $x_1$ direction, that vanishes as $|x_3|\to\infty$, and satisfies the boundary conditions

$$\varphi(x_1x_3\,|\,\omega)\big|_{x_3=\zeta(x_1)^-}=\varphi(x_1x_3\,|\,\omega)\big|_{x_3=\zeta(x_1)^+}\,, \tag{1.2a}$$

$$\epsilon(\omega)\frac{\partial}{\partial n_+}\varphi(x_1x_3\,|\,\omega)\big|_{x_3=\zeta(x_1)^-}=\frac{\partial}{\partial n_+}\varphi(x_1x_3\,|\,\omega)\big|_{x_3=\zeta(x_1)^+}\,. \tag{1.2b}$$

In Eq. (1.2b),

$$\frac{\partial}{\partial n_+}=\left[1+\left(\frac{d\zeta}{dx_1}\right)^2\right]^{-1/2}\left(-\frac{d\zeta}{dx_1}\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_3}\right) \tag{1.3a}$$

is the derivative along the unit vector directed normally outward from the surface, i.e., from the dielectric into the vacuum. We will also have occasion to use the normal derivative $\partial/\partial n_-$ that is defined by

$$\frac{\partial}{\partial n_-}\equiv-\frac{\partial}{\partial n_+}\,. \tag{1.3b}$$

We see from Eqs. (1.1) and (1.2) that there is no loss of generality in our assumption of a dielectric-vacuum interface. For, if the region $x_3>\zeta(x_1)$ were filled with a dielectric medium characterized by a dielectric constant $\epsilon_2(\omega)$, while if the region $x_3<\zeta(x_1)$ were filled with a dielectric whose dielectric constant was $\epsilon_1(\omega)$; the results obtained here could be applied to that case merely by replacing $\epsilon(\omega)$ with $\epsilon_1(\omega)/\epsilon_2(\omega)$.

In Sec. II we obtain the dispersion relation for surface plasmons on a grating on the basis of the Rayleigh hypothesis. This is the name given the assumption[6] that the solutions of Eq. (1.1) that are valid outside the selvedge region can be continued into the selvedge region, to the surface $x_3=\zeta(x_1)$ itself, and used in the boundary conditions (1.2). It is now known[7-9] that in the case of the scattering of a scalar plane wave from a corrugated hard wall described by the surface profile function

$$\zeta(x_1)=\zeta_0\cos\frac{2\pi x_1}{a}, \tag{1.4}$$

the Rayleigh hypothesis is valid provided the ratio $(\zeta_0/a)<0.072$. The limits of validity of the Rayleigh hypothesis are not known for the problem we are studying in this paper. However, it can be safely assumed that it is valid only for a sufficiently small degree of surface roughness. Nevertheless, the derivation of the surface-plasmon dispersion relation on the basis of the Rayleigh hypothesis is a simple one, and the results obtained through its use are exact in the small roughness limit.

In Sec. III an exact dispersion relation for surface plasmons on a grating is obtained by the use of the extinction-theorem form of Green's theorem. The extinction-theorem formulation, as followed here, is presented by Toigo *et al.*[10] for the case of the scattering of an electromagnetic wave from the periodically rough surface. It is free from the limitations present in the use of the Rayleigh hypothesis and enables quite rough surfaces to be studied. This same extinction-theorem method of Ref. 10 was also followed by Laks *et al.*[11] to calculate the dispersion relation of surface polaritons (i.e., with retardation).

Numerical results for the dispersion curves obtained by both the Rayleigh and extinction-theorem methods will be described for two different surface profiles in Sec. IV, and a brief discussion of the results obtained and conclusions that can be drawn from them will be presented in Sec. V.

## II. THE RAYLEIGH HYPOTHESIS

In this section we solve the boundary-value problem posed by Eqs. (1.1)–(1.2) on the basis of the Rayleigh hypothesis.[6-9] The solution of Eq. (1.1) that vanishes as $x_3\to+\infty$ can be written for $x_3>\zeta_{\max}$ in the form

$$\varphi^{>}(x_1x_3\,|\,\omega)=\sum_{p=-\infty}^{\infty}A_p\exp(ik_px_1-|k_p|x_3), \tag{2.1}$$

where

$$k_p=k+\frac{2\pi p}{a}, \tag{2.2}$$

and $k$ is the wave vector of the plasmon. Similarly, the solution of Eq. (1.1) that vanishes as $x_3\to-\infty$ can be written for $x_3<\zeta_{\min}$ in the form

$$\varphi^{<}(x_1x_3\,|\,\omega)=\sum_{p=-\infty}^{\infty}B_p\exp(ik_px_1+|k_p|x_3). \tag{2.3}$$

Both solutions possess the Bloch property

$$\varphi(x_1+a,x_3\,|\,\omega)=e^{ika}\varphi(x_1x_3\,|\,\omega), \tag{2.4}$$

as they must in view of the periodicity of the surface profile function.

We now assume that the solutions (2.1) and (2.3) can be continued into the surface itself (this is the Rayleigh hypothesis), and substitute them into the boundary conditions (1.2). The expansion coefficients $\{A_p\}$ and $\{B_p\}$ are thereby found to satisfy the pair of homogeneous equations

$$\sum_{p=-\infty}^{\infty}\left(-e^{-|k_p|\zeta(x_1)+ik_px_1}A_p+e^{|k_p|\zeta(x_1)+ik_px_1}B_p\right)=0, \tag{2.5a}$$

$$\sum_{p=-\infty}^{\infty}\Bigg[\left(|k_p|+ik_p\frac{d\zeta(x_1)}{dx_1}\right)e^{-|k_p|\zeta(x_1)+ik_px_1}A_p+\epsilon(\omega)\left(|k_p|-ik_p\frac{d\zeta(x_1)}{dx_1}\right)\times e^{|k_p|\zeta(x_1)+ik_px_1}B_p\Bigg]=0. \tag{2.5b}$$

Past this point one can proceed in several alternative ways to obtain the dispersion relation for surface plasmons.[12] We proceed here in a manner that leads to a form for the dispersion relation well suited for numerical calculations. We multiply Eq. (2.5a) by $[|k_r|+ik_r d\zeta(x_1)/dx_1]\times\exp[|k_r|\zeta(x_1)-ik_rx_1]$, multiply Eq. (2.5b) by $-\epsilon^{-1}(\omega)\exp[|k_r|\zeta(x_1)-ik_rx_1]$, add the resulting equations, and integrate the sum on $x_1$ over the interval $(-\frac{1}{2}a,\frac{1}{2}a)$. In this way we obtain an equation for the $\{A_p\}$ alone:

$$\sum_{p=-\infty}^{\infty}\frac{1}{a}\int_{-a/2}^{a/2}dx_1\left([\epsilon(\omega)|k_r|+|k_p|]+i[\epsilon(\omega)k_r+k_p]\frac{d\zeta(x_1)}{dx_1}\right)\exp[(|k_r|-|k_p|)\zeta(x_1)-i(k_r-k_p)x_1]A_p=0. \tag{2.6}$$

An equation of this type for surface polaritons was first obtained by Toigo *et al.*[10]

The term containing $d\zeta(x_1)/dx_1$ can be integrated by parts. It yields a nonzero contribution only for $p\neq r$ on the assumption, that we make here, that $\zeta(\frac{1}{2}a)^-=\zeta(-\frac{1}{2}a)^+$. This assumption means that in addition to being periodic in $x_1$ with period $a$, $\zeta(x_1)$ has no jump discontinuities at $x_1=\pm a/2$, or within the interval $-(a/2)\leq x_1\leq(a/2)$. The modifications in the results that follow when this is not the case are straightforward. Thus Eq. (2.6) can be rewritten as

$$\sum_{p=-\infty}^{\infty}\left(\delta_{rp}[\epsilon(\omega)+1]|k_r|+(1-\delta_{rp})[1-\epsilon(\omega)]\frac{|k_r||k_p|-k_rk_p}{|k_r|-|k_p|}\frac{1}{a}\int_{-a/2}^{a/2}dx_1e^{(|k_r|-|k_p|)\zeta(x_1)}e^{-i(k_r-k_p)x_1}\right)A_p=0. \tag{2.7}$$

This equation can be rearranged into the form

$$\sum_{p=-\infty}^{\infty} M_{rp}(k)A_p = \frac{\epsilon(\omega)+1}{\epsilon(\omega)-1} A_r , \tag{2.8}$$

where the elements of the matrix $\tilde{M}(k)$ are given by

$$M_{rp}(k) = \begin{cases} \dfrac{|k_r|k_p| - k_r k_p}{|k_r|(|k_r| - |k_p|)} \dfrac{1}{a} \displaystyle\int_{-a/2}^{a/2} dx_1 e^{(|k_r|-|k_p|)\zeta(x_1)} e^{-i(2\pi/a)(r-p)x_1}, & r \neq p & (2.9a) \\ 0, \quad r = p . & & (2.9b) \end{cases}$$

Consequently, if we denote the eigenvalues of the matrix $\tilde{M}(k)$ by $\{\lambda_s(k)\}$, where $s$ labels the distinct eigenvalues, the dispersion relation for a surface plasmon on a grating can be written as

$$\frac{\epsilon(\omega)+1}{\epsilon(\omega)-1} = \lambda_s(k) , \tag{2.10}$$

and leads to a separate branch for each distinct eigenvalue.

The eigenvalues $\{\lambda_s(k)\}$ are periodic functions of $k$ with period $2\pi/a$. This can be seen as follows. If we replace $k$ by $k + 2\pi/a$ in the expression for the matrix element $M_{rp}(k)$ given by Eq. (2.9), this has the effect of replacing $k_r$ by $k_{r+1}$ and $k_p$ by $k_{p+1}$, according to Eq. (2.2). Consequently, we have the result

$$M_{rp}(k + (2\pi/a)) = M_{r+1,\, p+1}(k) = M_{r',p'}(k) , \tag{2.11}$$

where $r' = r+1$, $p' = p+1$. The relabeling of rows and columns of an infinite matrix in this way leaves the eigenvalues unaltered, and we therefore have the result

$$\lambda_s(k + (2\pi/a)) = \lambda_s(k) . \tag{2.12}$$

As a result of Eq. (2.12) we can restrict $k$ to lie in the interval of $0 \leqslant k \leqslant (2\pi/a)$ with no loss of generality. The numerical solution of Eqs. (2.9)–(2.10) will be discussed in Sec. IV.

We now turn to a determination of a dispersion relation for surface plasmons that is free from the limitations of the Rayleigh hypothesis.

## III. THE EXTINCTION-THEOREM METHOD

To obtain a dispersion relation for surface plasmons on a grating that is free from the limitations of the Rayleigh hypothesis, we begin with Green's theorem[13] and follow the methodology of Ref. 10. If $u(\vec{x})$ and $v(\vec{x})$ are arbitrary scalar fields defined in the volume $V$ bounded by the closed surface $\Sigma$, this theorem states that

$$\int_V (u\nabla^2 v - v\nabla^2 u) d^3x = \int_\Sigma \left( u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right) dS , \tag{3.1}$$

where $\partial/\partial n$ is the normal derivative at the surface $\Sigma$, directed outward from inside the volume $V$.

If we apply Eq. (3.1) to the vacuum above the dielectric medium, we obtain the pair of equations

$$-\frac{1}{4\pi}\int_S \left(\frac{\partial}{\partial n'_-} G(x_1x_3|x'_1x'_3)\varphi^{>}(x'_1x'_3|\omega) - G(x_1x_3|x'_1x'_3)\frac{\partial}{\partial n'_-}\varphi^{>}(x'_1x'_3|\omega)\right) ds'_1 = \begin{cases} \varphi^{>}(x_1x_3|\omega) , & x_3 > \zeta(x_1) & (3.2a) \\ 0, & x_3 < \zeta(x_1) . & (3.2b) \end{cases}$$

In Eqs. (3.2) $\varphi^{>}(x_1x_3|\omega)$ is the electrostatic potential in the region $x_3 \geqslant \zeta(x_1)$, and $G(x_1x_3|x'_1x'_3)$ is a Green's function that is the solution of

$$\nabla^2 G(x_1x_3|x'_1x'_3) = -4\pi\,\delta(x_1 - x'_1)\delta(x_3 - x'_3) . \tag{3.3}$$

The Fourier integral representation of this function is

$$G(x_1x_3|x'_1x'_3) = \int_{-\infty}^{\infty} dq \frac{\exp[iq(x_1 - x'_1) - |q||x_3 - x'_3|]}{|q|} . \tag{3.4}$$

The integration in Eq. (3.2) is carried out over the corrugated dielectric-vacuum interface, and $ds'_1$ is the element of path length along this surface. Because we seek solutions $\varphi^{>}(x_1x_3|\omega)$ that vanish as $x_3 \to \infty$, there is no contribution to the left-hand side of Eq. (3.2) from the surface of an infinite hemisphere in the upper half-space that together with the surface $S$ constitutes the surface $\Sigma$.

If we now apply Eq. (3.1) to the region occupied by the dielectric medium, we obtain the following pair of equations:

$$-\frac{1}{4\pi}\int_S \left(\frac{\partial}{\partial n'_+} G(x_1x_3|x'_1x'_3)\varphi^{<}(x'_1x'_3|\omega) - G(x_1x_3|x'_1x'_3)\frac{\partial}{\partial n'_+}\varphi^{<}(x'_1x'_3|\omega)\right) ds'_1 = \begin{cases} 0, & x_3 > \zeta(x_1) & (3.5a) \\ \varphi^{<}(x_1x_3|\omega), & x_3 < \zeta(x_1) . & (3.5b) \end{cases}$$

In Eqs. (3.5) $\varphi^<(x_1'x_3'|\omega)$ is the electrostatic potential in the region $x_3 \leq \zeta(x_1)$. If we make use of the boundary conditions (1.2), as well as the relation (1.3b), we can transform Eqs. (3.5) into

$$\frac{1}{4\pi}\int_S\left(\frac{\partial}{\partial n_-'}G(x_1x_3|x_1'x_3')\varphi^>(x_1'x_3'|\omega)-\epsilon(\omega)^{-1}G(x_1x_3|x_1'x_3')\frac{\partial}{\partial n_-'}\varphi^>(x_1'x_3'|\omega)\right)ds_1' = \begin{cases}0, & x_3>\zeta(x_1) \quad (3.6a)\\ \varphi^<(x_1x_3|\omega), & x_3<\zeta(x_1). \quad (3.6b)\end{cases}$$

Although one can obtain more than one form of the dispersion relation for surface plasmons on a grating by starting from Eqs. (3.2) and (3.6),[12] the procedure we will follow here yields a particularly simple form of this relation. We begin by expressing the element of integration $ds_1$ in terms of $dx_1$ alone, in the integrals over the surface $S$ on the left-hand sides of Eqs. (3.2) and (3.6). For this we use

$$ds_1=\left[1+\left(\frac{d\zeta}{dx_1}\right)^2\right]^{1/2}dx_1\,, \tag{3.7}$$

and the definition (1.3), and obtain the two pairs of equations

$$-\frac{1}{4\pi}\int dx_1'\left[\left(\frac{d\zeta}{dx_1'}\frac{\partial}{\partial x_1'}-\frac{\partial}{\partial x_3'}\right)G(x_1x_3|x_1'x_3')H(x_1'|\omega)-G(x_1x_3|x_1'x_3')L(x_1'|\omega)\right]_{x_3'=\zeta(x_1')} = \begin{cases}\varphi^>(x_1x_3|\omega), & x_3>\zeta(x_1) \quad (3.8a)\\ 0, & x_3<\zeta(x_1) \quad (3.8b)\end{cases}$$

$$\frac{1}{4\pi}\int dx_1'\left[\left(\frac{d\zeta}{dx_1'}\frac{\partial}{\partial x_1'}-\frac{\partial}{\partial x_3'}\right)G(x_1x_3|x_1'x_3')H(x_1'|\omega)-\epsilon(\omega)^{-1}G(x_1x_3|x_1'x_3')L(x_1'|\omega)\right]_{x_3'=\zeta(x_1')} = \begin{cases}0, & x_3>\zeta(x_1)\\ \varphi^<(x_1x_3|\omega), & x_3<\zeta(x_1)\end{cases}$$

(3.9a)

(3.9b)

where

$$H(x_1|\omega)=\varphi^>(x_1x_3|\omega)|_{x_3=\zeta(x_1)}\,, \tag{3.10a}$$

$$L(x_1|\omega)=\left[1+\left(\frac{d\zeta}{dx_1}\right)^2\right]^{1/2}\frac{\partial}{\partial n_-}\varphi^>(x_1x_3|\omega)|_{x_3=\zeta(x_1)}\,. \tag{3.10b}$$

Equation (3.8b) holds for all $x_3<\zeta(x_1)$. We will require that it be satisfied for any value of $x_3<\zeta_{\min}$. Similarly, Eq. (3.9a) holds for all $x_3>\zeta(x_1)$. We will require that it be satisfied for any value of $x_3>\zeta_{\max}$. We then substitute into these two equations the Fourier integral representation of the Green's function $G(x_1x_3|x_1'x_3')$ given by Eq. (3.4), and use the periodicity of $\zeta(x_1)$ and the Bloch property of $H(x_1|\omega)$ and $L(x_1|\omega)$,

$$H(x_1+a|\omega)=e^{ika}H(x_1|\omega)\,, \tag{3.11a}$$

$$L(x_1+a|\omega)=e^{ika}L(x_1|\omega)\,, \tag{3.11b}$$

where $k$ is the plasmon wave vector. In this way we obtain the following pair of coupled homogeneous equations for $H(x_1|\omega)$ and $L(x_1|\omega)$:

$$\frac{1}{a}\int_{-a/2}^{a/2}dx_1 e^{-ik_mx_1-|k_m|\zeta(x_1)}\{[ik_m\zeta'(x_1)-|k_m|]H(x_1|\omega)+L(x_1|\omega)\}=0 \quad \text{for each } m\,, \tag{3.12a}$$

$$\frac{1}{a}\int_{-a/2}^{a/2}dx_1 e^{-ik_mx_1+|k_m|\zeta(x_1)}\{[ik_m\zeta'(x_1)+|k_m|]H(x_1|\omega)+\epsilon(\omega)^{-1}L(x_1|\omega)\}=0 \quad \text{for each } m\,. \tag{3.12b}$$

To solve this pair of equations we expand $H(x_1|\omega)$ and $L(x_1|\omega)$ in Fourier series according to

$$H(x_1|\omega)=\sum_{n=-\infty}^{\infty}e^{ik_nx_1}\hat{H}_n(k\omega)\,, \tag{3.13a}$$

$$L(x_1|\omega)=\sum_{n=-\infty}^{\infty}e^{ik_nx_1}\hat{L}_n(k\omega)\,, \tag{3.13b}$$

and substitute these expansions into Eqs. (3.12); the equations for the Fourier coefficients take the simple forms

$$\sum_{n=-\infty}^{\infty} I_{m-n}^{(m)}(k)\left(\frac{k_m k_n}{|k_m|}\hat{H}_n(k\omega) - \hat{L}_n(k\omega)\right) = 0\,, \tag{3.14a}$$

$$\sum_{n=-\infty}^{\infty} J_{m-n}^{(m)}(k)\left(\epsilon(\omega)\frac{k_m k_n}{|k_m|}\hat{H}_n(k\omega) + \hat{L}_n(k\omega)\right) = 0\,, \tag{3.14b}$$

where

$$I_n^{(m)}(k) = \frac{1}{a}\int_{-a/2}^{a/2} dx_1 e^{-i(2\pi n/a)x_1} e^{-|k_m|\zeta(x_1)}\,, \tag{3.15a}$$

$$J_n^{(m)}(k) = \frac{1}{a}\int_{-a/2}^{a/2} dx_1 e^{-i(2\pi n/a)x_1} e^{|k_m|\zeta(x_1)}\,. \tag{3.15b}$$

The two corresponding equations for polaritons (2.25) in Ref. 11 (to be called LMM) can be shown to be equivalent to our Eqs. (3.14) in the electrostatic limit if after letting $c \to \infty$, we multiply both equations (2.25) by $|k_m|/k_m = k_m/|k_m|$, multiply (2.25b) by $\epsilon(\omega)$, and then use the substitutions

$$k_n \hat{H}_n^{(\mathrm{LMM})} = \hat{L}_n$$

and

$$\hat{L}_n^{(\mathrm{LMM})} = k_n \hat{H}_n\,.$$

The $\hat{H}_n$ and $\hat{L}_n$ reverse roles in the two problems, because in one case they refer to a component of the vector magnetic field and in the other case to the electric scalar potential.

The dispersion relation for surface plasmons on a grating is obtained by equating to zero the determinant of the coefficients in these equations (3.14). It is known from the theory of a related problem, viz., the scattering of a scalar plane wave by a periodically corrugated hard wall,[14] that Eqs. (3.12) are exact, but that their solution by Fourier series as we have done here may not converge for surface profile functions $\zeta(x_1)$ of sufficiently large amplitude. Nevertheless, we will see in the following section that at least for an analytic profile function, the solution of Eqs. (3.14) yields convergent results for the surface plasmon dispersion curve for quite large amplitudes of the corrugation.

## IV. NUMERICAL RESULTS

In this section we describe the numerical solution of the dispersion relations derived in Secs. II and III in the case that the dielectric medium on which the grating is ruled is a free-electron metal, whose dielectric constant is

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}\,, \tag{4.1}$$

where $\omega_p$ is the bulk plasma frequency of the conduction electrons in the metal.

Two different surface profiles have been used in these calculations. The first is the sinusoidal profile given by

$$\zeta(x_1) = \zeta_0 \cos\frac{2\pi x_1}{a}\,. \tag{4.2}$$

The second is the symmetric sawtooth profile, defined by

$$\zeta(x_1) = \begin{cases} h + \dfrac{4h}{a}x_1, & -\dfrac{a}{2} \le x_1 \le 0 \quad (4.3a)\\[2mm] h - \dfrac{4h}{a}x_1, & 0 \le x_1 \le \dfrac{a}{2}\,. \quad (4.3b)\end{cases}$$

Whether it is the Rayleigh method or the method based on Green's theorem, the following integral is required for each choice of the surface profile function $\zeta(x_1)$:

$$I = \frac{1}{a}\int_{-a/2}^{a/2} dx_1 e^{-i(2\pi n/a)x_1} e^{\alpha\zeta(x_1)}\,. \tag{4.4}$$

This integral can be evaluated analytically for each of the profiles given by Eqs. (4.2) and (4.3), and the results are as follows.

*Sinusoidal:*

$$I = I_n(\zeta_0\alpha)\,, \tag{4.5}$$

where $I_n(x)$ is a modified Bessel function.

*Sawtooth:*

$$I = \begin{cases} \dfrac{4h\alpha}{\pi^2 n^2 + 4h^2\alpha^2}\sinh h\alpha, & n \text{ even} \quad (4.6a)\\[2mm] \dfrac{4h\alpha}{\pi^2 n^2 + 4h^2\alpha^2}\cosh h\alpha, & n \text{ odd.} \quad (4.6b)\end{cases}$$

We now consider in turn the numerical solution of the dispersion relations given by Eqs. (2.9)–(2.10) and Eqs. (3.14)–(3.15).

### A. The Rayleigh hypothesis

With the choice of dielectric function given by Eq. (4.1), the dispersion relation for surface plasmons that follows from Eq. (2.10) of the Rayleigh method can be written

$$\omega(k) = \frac{\omega_p}{\sqrt{2}}[1 - \lambda_s(k)]^{1/2}\,. \tag{4.7}$$

The solution for the eigenvalues, $\lambda_s(k)$, of the infinite matrix $\tilde{M}(k)$ is found, for a fixed $k$, by diagonalizing a matrix of finite dimension, $N$ [corresponding to $r$, $p = -N/2, \ldots, 0, \ldots, N/2 - 1$ in Eqs. (2.9)], and searching for a converging result as $N$ is increased.

For the sinusoidal profile, the eigenvalues occur in pairs: $\pm\lambda_1(k)$, $\pm\lambda_2(k), \ldots$, corresponding to branches of the dispersion relation that are shifted upward and downward nearly symmetrically with respect to the dispersionless flat-surface-plasmon dispersion curve at $\omega = \omega_p/\sqrt{2}$. The

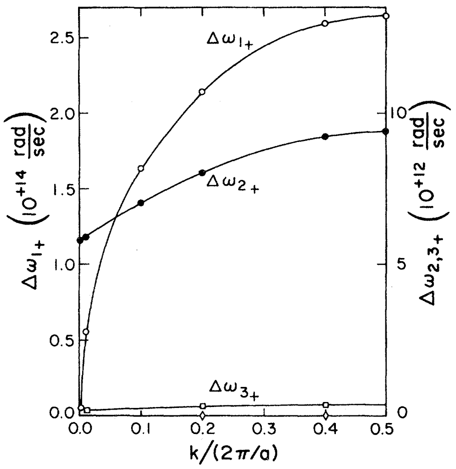


FIG. 1. Branches of the dispersion relation that are above the flat-surface-plasmon frequency, $\omega=\omega_p/\sqrt{2}$, for a sinusoidal profile with $\zeta_0/a=0.07$. Measured from $\omega_p/\sqrt{2}$ as $\Delta\omega_{s+}(k)$ and calculated with the Rayleigh method: ○—$\Delta\omega_{1+}$, ●—$\Delta\omega_{2+}$, □—$\Delta\omega_{3+}$, and ◇—$\Delta\omega_{s+}$ for $s>3$ (taking $\hbar\omega_p=15.3$ eV for Al).

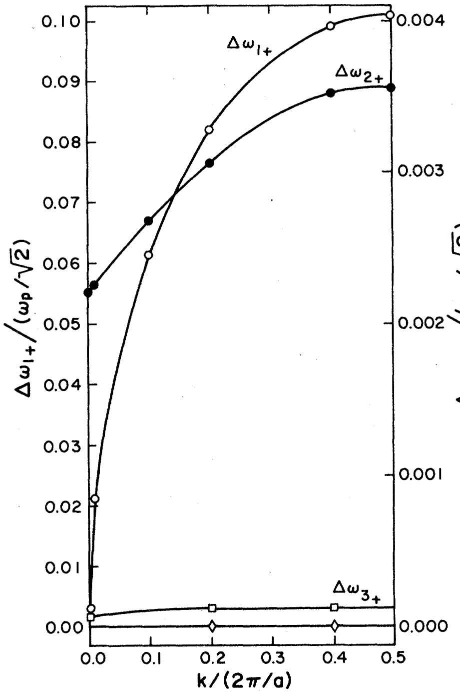


FIG. 2. The $\ln|\Delta\omega_{s-}|$ vs the $\ln\zeta_0/a$ at $k=0.2$ $(2\pi/a)$ for a sinusoidal profile, for the three branches the farthest below the flat-surface-plasmon frequency: (1) $\Delta\omega_{1-}$, (2) $\Delta\omega_{2-}$, and (3) $\Delta\omega_{3-}$. Here $\hbar\omega_p=15.3$ eV corresponding to Al, and ○—Rayleigh method and □—Green's-theorem method.

difference between this frequency of the flat-surface plasmon and that of a branch of $\omega(k)$ is expressed as

$$\Delta\omega_{s\pm}(k)=\frac{\omega_p}{\sqrt{2}}[1\pm\lambda_s(k)]^{1/2}-\frac{\omega_p}{\sqrt{2}}. \tag{4.8}$$

In Fig. 1 we have plotted $\Delta\omega_{s+}(k)$ for the case that $\zeta_0/a=0.07$ (not shown is the fact that the dispersion curve is symmetric with respect to $k=0$. The eigenvalues $\{\lambda_s(k)\}$ decrease in magnitude essentially geometrically: $|\lambda_1|>|\lambda_2|>|\lambda_3|>\cdots$, with $|\lambda_s|/|\lambda_{s+1}|\approx$const, so that the branches rapidly merge into the flat-surface curve as $|\lambda_s|\to 0$.

Convergence with increasing $N$ is always most rapid for $\pm\lambda_1(k)$, the largest eigenvalue pair, and becomes slower for each successively smaller $\lambda_s$. Moreover, the convergence becomes slower as the ratio $\zeta_0/a$ is increased.

Beginning at the ratio $\zeta_0/a=0.016$ and using matrices up to $N=48$, we find clear convergence down to the tenth pair of eigenvalues for $\zeta_0/a$ up to 0.07, down to the seventh pair for $\zeta_0/a$ up to 0.075, and to the third pair for $\zeta_0/a$ up to 0.1 (with values nearly identical to those found with the extinction-theorem method to be discussed below). At $\zeta_0/a=0.116$, divergence is seen in the largest eigenvalue pairs. Divergence for a value of $\zeta_0/a$ smaller than 0.116 may be seen in the very small eigenvalues; for example, at $\zeta_0/a=0.1$ the $\pm\lambda_5$ are diverging. It is, however, often difficult to interpret the convergence properties of the small eigenvalues. This is because spurious results, such as degeneracies (with nonzero imaginary parts), occur in them, even at small $\zeta_0/a$, but more frequently as $\zeta_0/a$ is increased.

It is, furthermore, interesting to note that $|\Delta\omega_{1\pm}|$ is directly proportional to $\zeta_0/a$, $|\Delta\omega_{2\pm}|$ to $(\zeta_0/a)^3$, $|\Delta\omega_{3\pm}|$ to $(\zeta_0/a)^5$, etc. (see Fig. 2). This is what we find analytically for $\Delta\omega_1$ and $\Delta\omega_2$ when we expand the exponential in the integral of Eqs. (2.9) to $O(\zeta^3(x_1))$ in the small roughness limit.

For the sawtooth profile, Eqs. (4.3), the Rayleigh method again yields pairs of eigenvalues: $\pm\lambda_1(k)$, $\pm\lambda_2(k),\ldots$, which for the small ratio $h/a=0.016$ are each tending towards convergence as we increase $N$ up to about 30. Moreover, these $\lambda_s(k)$ when calculated with small $N$ matrices yield dispersion curves that are nearly identical to those found with the extinction-theorem approach. However, as $N$ is increased beyond 30, the eigenvalues all begin to diverge. This behavior is reminiscent of the conclusion by Hill and Celli,[9] for the scattering of a plane wave from a corrugated surface, namely, that the Rayleigh method is valid when a nonanalytic profile is approximated by its Fourier series up to a certain number of terms, beyond which the method becomes invalid. At larger $h/a$, e.g., $h/a=0.064$, the eigenvalues, $\lambda_s(k)$, are seen to be diverging and to have nonzero imaginary parts beginning immediately with small $N$.

### B. Extinction theorem

The solutions, $\omega_s(k)$, that are the zeros of the infinite-dimensional determinant of the coefficients in Eqs. (3.14), are found by solving the $N$-dimensional determinant equation [corresponding to $m$, $n=-(N/4-1),\ldots,0,\ldots,N/4$] and searching for convergence as $N$ is increased. The $N$-dimensional determinant equation yields $N/4-1$ pairs of roots, corresponding to the branches of the dispersion relation found with the Rayleigh method. Because these branches rapidly merge into the flat-surface curve, $\omega=\omega_p/\sqrt{2}$, only a few may be resolved by a numerical root search, thus demonstrating a computational advantage of the Rayleigh method, which immediately yields all $N/2$ pairs of branches.

For the sinusoidal profile, using matrices of dimension up to $N=48$, we have convergent results for ratios of $\zeta_0/a$ up to 0.25, while at $\zeta_0/a=0.3$ we begin to see nonconvergent behavior. The limit of $\zeta_0/a=0.116$, where the Rayleigh method gives a diverging $\lambda_1$, is now seen to be the point where the plots of $\ln\zeta_0/a$ vs $\ln\Delta\omega$ no longer follow straight lines (Fig. 2). The curves of $\Delta\omega(k)$ for $\zeta_0/a=0.25$ are plotted in Fig. 3.

For the sawtooth profile, for a ratio of $h/a=0.016$ using determinants of up to $N=48$, we have investigated the first three branches and have found convergence. Convergence is also seen for $h/a=0.04$. However, divergence is found when $h/a\geq 0.064$.

The present results for the surface-plasmon dispersion curves obtained by use of the extinction theorem may be compared to those in the work of Laks *et al.* for a surface polariton on a grating,[11] which uses a similar extinction-theorem approach but proceeds from Maxwell's equations and thus includes retardation. For large $k$ where the flat-surface polariton becomes almost dispersionless, the two sets of results should agree. Indeed, in this limit the three pairs of branches about $\omega_p/\sqrt{2}$ for a sinusoidal grating that are considered in Ref. 11 have frequency spacings corresponding to the first three pairs of branches found here.

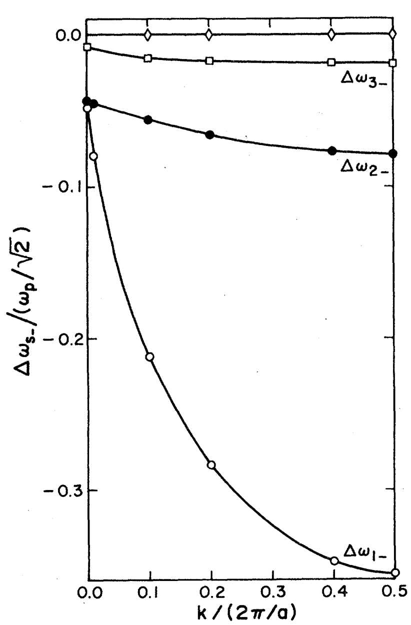


FIG. 3. Branches of the dispersion relation that are below the flat-surface-plasmon frequency, $\omega=\omega_p/\sqrt{2}$, for a sinusoidal profile with $\zeta_0/a=0.25$. Measured from $\omega_p/\sqrt{2}$ as $\Delta\omega_{s-}(k)$ and calculated with the Green's theorem method: ○—$\Delta\omega_{1-}$, ●—$\Delta\omega_{2-}$, □—$\Delta\omega_{3-}$, and ◇—$\Delta\omega_{s-}$ with $s>3$ (taking $\hbar\omega_p=15.3$ eV for Al).

## V. CONCLUSIONS

Both a method based upon the Rayleigh approximation and a formally exact method based upon the extinction theorem, with Fourier expansions of the terms containing the unknown scalar field and its normal derivative on the boundary, predict the existence of an infinite series of branches in the dispersion relation of a plasmon propagating on a surface with periodic roughness. No more than, perhaps, two or three of these branches will be experimentally resolvable, since they merge rapidly into the flat-surface-plasmon curve at $\omega=\omega_p/\sqrt{2}$. To heighten their resolution, a very large roughness will be desirable, as their separation, $\Delta\omega(k)$, from $\omega_p/\sqrt{2}$ is proportional to some power of the roughness strength.

For the purpose of computation, the Rayleigh method is the easier one, directly yielding $N$ branches when formulated as an $N$-dimensional-matrix eigenvalue problem. It is, however, valid only for small roughness ($\zeta_0/a\lesssim 0.1$) when applied to an analytic profile, and even more restricted when applied to a nonanalytic profile.

The extinction-theorem method, with a Fourier expansion, yields properly convergent results for the plasmon dispersion relation with much larger roughness strengths. When used with a sinusoidal profile, it leads to no problem with ill-conditioned matrices, with profiles with $\zeta_0/a$ up to 0.25. Results for the nonanalytic sawtooth profile, for relatively small roughness, are also found to be convergent—here, ill-conditioned matrices arise for $\zeta_0/a\geq 0.064$.

We emphasize the fact that the extinction-theorem method is formally exact, the lack of convergence for large roughness being due to expansions in Fourier series. Expansion in a different set of basis functions could lead to convergence where the Fourier expansion does not.[12,14]

It is hoped that the results presented here for periodic profiles, valid for very large roughness strengths, may also provide insight into the properties of the surface-plasmon dispersion curve for a randomly rough surface with large roughness strengths. In particular, one can speculate that more than the two branches obtained in Refs. 3 and 4 in the small roughness limit will be found in this case in the limit of large roughness.

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