Effects of surface roughness on the surface-polariton dispersion relation

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The effects of surface roughness on the dispersion relation for surface polaritons at the rough interface between vacuum and a semi-infinite dielectric medium, characterized by an isotropic dielectric constant $\epsilon(\omega)$, have been determined. An integral equation is established for the Green's function for the matrix differential operator in Maxwell's equation for the macroscopic electric field in the presence of a rough interface, in terms of the corresponding Green's function in the presence of a plane interface. On the assumption that the Fourier coefficients of the surface roughness profile function are Gaussianly distributed random variables the integral equation can be solved. The position of the pole in the resulting solution corresponding to the frequency of the surface polariton has been determined through terms of $O(\delta^2)$, where δ^2 is the mean-square deviation of the surface from flatness. The resulting expressions for the real and imaginary parts of the surface-polariton dispersion relation are evaluated for two different choices of $\epsilon(\omega)$, the first corresponding to a diatomic polar crystal of cubic symmetry, the second corresponding to intraband transitions in a metal or semiconductor with free carriers. The effects of surface roughness are found to be significant only for wavelengths of the surface polariton comparable with or longer than the transverse correlation length characterizing the horizontal distribution of surface roughness.

I. INTRODUCTION

It is now well known that any electric dipole active excitation in a solid, which contributes a pole to its dielectric tensor, can couple linearly to the electromagnetic field in the solid to produce as the normal modes of the system excitations called polaritons.[1,2] If the solid is semi-infinite, and is terminated by a planar boundary separating it from the vacuum outside, which will be the case of interest in the present work, these polaritons can be bound to the solid-vacuum interface, and are then called surface polaritons.[2-4] The electromagnetic field associated with a surface polariton is wavelike in directions parallel to the interface, but its amplitude decays exponentially with increasing distance into the solid and into the vacuum away from the interface. Various properties of surface polaritons have now been studied both theoretically and experimentally.[2-4]

As a surface polariton propagates along a solid-vacuum interface it is attenuated. The mechanisms responsible for this attenuation can be described as intrinsic and extrinsic. By intrinsic we mean the dissipative processes present in the bulk of the solid, i.e., the processes which give rise to the imaginary part of the dielectric tensor. In insulators and semiconductors, for frequencies in the infrared, these can be the anharmonic interactions of the normal modes of vibration; in semiconductors and metals these can be interband electronic transitions. By extrinsic mechanisms for the attenuation of surface polaritons we mean such things as the presence of point defects in the vicinity of the surface of the solid, or surface roughness, which can scatter the surface polariton as it progresses along the interface and thereby remove energy from the incident beam.

The attenuation of surface polaritons by intrinsic processes is readily determined by substituting the complex dielectric constant of the solid into the dispersion relation for these modes, and solving it for the imaginary part of the wave vector of the surface polariton, which is half the inverse attenuation length of the surface polariton.[5] The result so obtained is in good agreement with existing experimental data.[5,6]

The attenuation mechanisms we have labeled extrinsic are specific to the surface region of the solid, and are little studied, either theoretically or experimentally. Notwithstanding the fact that the surfaces of solids used in the infrared and optical frequency ranges are carefully prepared, many surface preparation techniques leave a residual surface roughness whose horizontal and vertical scale can be of the order of a few hundred angstroms. It is therefore of some interest to determine the effect of this surface roughness on the frequency and damping of surface polaritons.

In a recent paper Mills[7] has studied the contribution to the linewidth and attenuation length of surface polaritons arising from surface roughness. By treating the surface roughness as a perturbation which scatters an incident surface polariton Mills calculated the scattered electromagnetic fields in both the solid and the vacuum outside it in first Born approximation, using a Green's-function approach which had been used earlier in studies of the scattering and absorption of electromagnetic radiation by the rough surface of a semi-infinite dielectric medium.[8,9] The contribution to the attenuation length and linewidth of the surface polariton from each of these scattered fields was obtained, and their relative importance examined, for surface polaritons in the infrared on semiconductor surfaces and on the surface of a nearly-free-electron metal. It was found that for physically reasonable values of the two parameters that characterize the surface roughness, viz, the root-mean-square deviation of the surface from flatness and the transverse correlation length, which is a measure of the average distance between successive "peaks" or "valleys" on the surface, the calculated attenuation lengths can be comparable with those observed experimentally.[5,6]

In this paper we present an alternative approach to that of Mills for the determination of the attenuation of surface polaritons by surface roughness. It is based on an operational definition of the attenuation in the following way.

The calculation of the cross section for the inelastic scattering of light from dipole-active excitations in a semi-infinite solid can be reduced to the evaluation of the Fourier transform with respect to time of the correlation function of the electric field in the system of solid plus the vacuum above it, $\langle E_\alpha(\vec{x},t)E_\beta(\vec{x}',t')\rangle$.[10] The angular brackets here denote an average with respect to an ensemble defined by the Hamiltonian of the solid and the electromagnetic field with which it interacts. It has been shown by Dzyaloshinski and Pitaevskii[11] (see also Ref. 8) that the required Fourier transform is very simply related to the Green's-function tensor for the partial differential operator, which appears in Maxwell's wave equation for the macroscopic electric field in the solid and the vacuum outside it. The elements of this tensor have been calculated for an isotropic dielectric medium bounded by a plane surface with vacuum outside.[8] As functions of frequency they possess a simple pole at the frequency $\omega=\omega_0(k_\parallel)$ of the surface polariton, which contributes a peak to the cross section for light scattering from this system at the frequency of the surface polariton. If the dielectric constant of the medium is taken to be real, the surface polariton peak in the scattering cross section is infinitely sharp (a δ function).

In this paper we calculate the elements of the Maxwell Green's-function tensor for an isotropic dielectric medium bounded by a rough surface with vacuum outside. An integral equation for the elements of this Green's-function tensor is obtained by treating the surface roughness as a perturbation on a perfectly flat surface, for which the corresponding Green's function is known. This integral equation is solved by iteration. With a certain assumption about the probability distribution function for the function describing the departure of the surface of the medium from flatness the resulting Neumann-Liouville series can be resummed (with the aid of a diagrammatic analysis) in terms of a proper self-energy, which is determined to lowest nonzero order in the surface profile function.

Examination of the elements of the Green's-function tensor obtained in this way reveals that as functions of frequency they possess a simple pole which is shifted from the frequency of the surface polariton associated with a planar solid-vacuum interface by a quantity which is proportional to δ^2 (the mean-square deviation of the surface from flatness), and is complex as well. The real part of this shift gives the surface-roughness-induced displacement of the position of the surface-polariton peak in the cross section for light scattering from the rough surface, or the change in the surface-polariton dispersion relation. The imaginary part of this shift gives the surface-roughness-induced linewidth of this peak, and is also related to the attenuation length of the surface polariton as it propagates along a rough surface.

Thus, the theory presented here yields the Maxwell Green's-function tensor which can be used to calculate the spectral distribution of light scattered inelastically from an isotropic, dielectric medium bounded by a rough surface. It yields the change in the dispersion relation of the surface polariton owing to surface roughness and it enables the attenuation length of the surface polariton owing to surface roughness to be calculated. It is found, just as in the work of Mills,[7] that two mechanisms give rise to the attenuation of surface polaritons by surface roughness: the polariton may radiate energy into the vacuum, or it may be scattered by the surface roughness into other surface-polariton states. The relative importance of both mechanisms is studied in the present work, and numerical results are presented for the attenuation length and frequency shift owing to surface roughness for surface polaritons in the infrared on semiconductor surfaces and on the surface of a nearly-free-electron metal.

II. GREEN'S FUNCTION FOR THE SCATTERING OF ELECTROMAGNETIC RADIATION BY A ROUGH SURFACE

In this section we obtain a formal result for the Green's function which describes the scattering of electromagnetic radiation from the rough surface of a dielectric medium. In Sec. III this result will be used to obtain the dispersion relation for surface polaritons in the presence of surface roughness.

We assume that the height of the surface of the dielectric medium above the xy plane is given by the equation

$$z=\zeta(x,y) . \tag{2.1}$$

Above this surface is vacuum, while the medium occupies the space below it, and is characterized by the (complex) frequency-dependent dielectric constant $\epsilon(\omega)$, which we assume to be isotropic. The dielectric constant of the system of medium plus the adjacent vacuum can be written

$$\epsilon(z;\omega)=\Theta(z-\zeta(x,y))+\epsilon(\omega)\Theta(\zeta(x,y)-z)\ , \tag{2.2}$$

where $\Theta(z)$ is Heaviside's unit step function. We now expand $\epsilon(z;\omega)$ to first order in $\zeta(x,y)$:

$$\epsilon(z;\omega)=\epsilon_0(z;\omega)+[\epsilon(\omega)-1]\zeta(x,y)\,\delta(z)+O(\zeta^2)\ , \tag{2.3}$$

where

$$\epsilon_0(z;\omega)=\begin{cases}1\ , & z>0\ ,\\ \epsilon(\omega)\ , & z<0\ .\end{cases} \tag{2.4}$$

If in Maxwell's equation

$$\nabla\times\nabla\vec{E}=-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{D} \tag{2.5}$$

we substitute

$$\vec{E}(\vec{x};t)=\vec{E}(\vec{x};\omega)\,e^{-i\omega t} \tag{2.6a}$$

$$\vec{D}(\vec{x};t)=\vec{D}(\vec{x};\omega)\,e^{-i\omega t}\ , \tag{2.6b}$$

and use the relation

$$\vec{D}(\vec{x};\omega)=\epsilon(z;\omega)\vec{E}(\vec{x};\omega)\ , \tag{2.7}$$

the equation for the Fourier coefficient of the electric field $\vec{E}(\vec{x};\omega)$ can be written in the form

$$\sum_\mu\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\lambda\mu}-\frac{\partial^2}{\partial x_\lambda\partial x_\mu}+\delta_{\lambda\mu}\nabla^2+[\epsilon(\omega)-1]\zeta(x,y)\,\delta(z)\frac{\omega^2}{c^2}\delta_{\lambda\mu}\right)E_\mu(\vec{x};\omega)=0\ . \tag{2.8}$$

We now define two Green's functions $\mathfrak{D}_{\mu\nu}(\vec{x},\vec{x}';\omega)$ and $D_{\mu\nu}(\vec{x},\vec{x}';\omega)$ as the solutions of the equations

$$\sum_\mu\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\lambda\mu}-\frac{\partial^2}{\partial x_\lambda\partial x_\mu}+\delta_{\lambda\mu}\nabla^2+[\epsilon(\omega)-1]\times\zeta(\vec{x}_\parallel)\,\delta(z)\frac{\omega^2}{c^2}\delta_{\lambda\mu}\right)\mathfrak{D}_{\mu\nu}(\vec{x},\vec{x}';\omega)=4\pi\delta_{\lambda\nu}\delta(\vec{x}-\vec{x}') \tag{2.9}$$

$$\sum_\mu\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\lambda\mu}-\frac{\partial^2}{\partial x_\lambda\partial x_\mu}+\delta_{\lambda\mu}\nabla^2\right)D_{\mu\nu}(\vec{x},\vec{x}';\omega)=4\pi\delta_{\lambda\nu}\,\delta(\vec{x}-\vec{x}')\ , \tag{2.10}$$

where $\vec{x}_\parallel=(x,y,0)$. The motivation for introducing these Green's functions is that it can be shown that the Fourier transforms with respect to time of electric field correlation functions such as appear in the cross section for light scattering can be expressed simply in terms of these functions.[8,10,11] Thus, the poles of the spatial Fourier transform of $\mathfrak{D}_{\mu\nu}(\vec{x},\vec{x}';\omega)$ as a function of ω give the frequencies of the excitations in the medium bounded by a rough surface from which the scattering occurs, among them the surface polaritons. Our program in this paper, therefore, will be to find the spatial Fourier transform of $\mathfrak{D}_{\mu\nu}(\vec{x},\vec{x}';\omega)$ and study that one of its poles whose frequency goes into that of a surface polariton when the surface profile function $\zeta(\vec{x}_\parallel)$ vanishes identically.

Equations (2.9) and (2.10) are to be solved subject to the boundary conditions that the solutions are either outgoing waves or damped as $z\to+\infty$, in addition to the usual electromagnetic boundary conditions of continuity of tangential $\vec{E}$ and $\vec{H}$ and normal $\vec{D}$ and $\vec{B}$ across the medium-vacuum interface. The Green's function $D_{\mu\nu}(\vec{x},\vec{x}';\omega)$ satisfies the latter conditions at the plane $z=0$; the Green's function $\mathfrak{D}_{\mu\nu}(\vec{x},\vec{x}';\omega)$ must satisfy them at the surface $z=\zeta(\vec{x}_\parallel)$. These two Green's functions are related by

$$\mathfrak{D}_{\lambda\nu}(\vec{x},\vec{x}';\omega)=D_{\lambda\nu}(\vec{x},\vec{x}';\omega)-\frac{\omega^2}{4\pi c^2}[\epsilon(\omega)-1]\times\sum_\mu\int d^3x''\,D_{\lambda\mu}(\vec{x},\vec{x}'';\omega)\,\zeta(\vec{x}_\parallel'')\,\delta(z'')\mathfrak{D}_{\mu\nu}(\vec{x}'',\vec{x}';\omega)\ . \tag{2.11}$$

The Green's function $D_{\lambda\nu}(\vec{x},\vec{x}'\omega)$ is known.[8] Our problem now is to solve Eq. (2.11) to obtain the unknown Green's function $\mathfrak{D}_{\lambda\nu}(\vec{x},\vec{x}';\omega)$ in terms of $D_{\lambda\nu}(\vec{x},\vec{x}';\omega)$.

We begin by simplifying Eq. (2.11). We Fourier analyze $\mathfrak{D}_{\lambda\nu}(\vec{x},\vec{x}';\omega)$ according to

$$\mathfrak{D}_{\lambda\nu}(\vec{x},\vec{x}';\omega)=\int\frac{d^2k_\parallel}{(2\pi)^2}\int\frac{d^2k_\parallel'}{(2\pi)^2}\times e^{i\vec{k}_\parallel\cdot\vec{x}_\parallel+i\vec{k}_\parallel'\cdot\vec{x}_\parallel'}\,\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega\,|\,zz')\ , \tag{2.12}$$

where $\vec{k}_\parallel=(k_x,k_y,0)$. The functions $D_{\lambda\nu}(\vec{x},\vec{x}';\omega)$ and $\zeta(\vec{x}_\parallel)$ can be Fourier analyzed according to[8]

$$D_{\lambda\nu}(\vec{x},\vec{x}',\omega)=\int\frac{d^2k_\parallel}{(2\pi)^2}\,e^{i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')}\,d_{\lambda\nu}(\vec{k}_\parallel\omega\,|\,zz')\ , \tag{2.13}$$

$$\zeta(\vec{x}_\parallel)=\int\frac{d^2k_\parallel}{(2\pi)^2}\,e^{i\vec{k}_\parallel\cdot\vec{x}_\parallel}\,\zeta(\vec{k}_\parallel)\ . \tag{2.14}$$

When we substitute Eqs. (2.12)–(2.14) into Eq. (2.11), we obtain the equation relating the Fourier coefficients $\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega\,|\,zz')$ and $d_{\lambda\nu}(\vec{k}_\parallel\omega\,|\,zz')$:

$$\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega\,|\,zz')=(2\pi)^2\delta(\vec{k}_\parallel+\vec{k}_\parallel')d_{\lambda\nu}(\vec{k}_\parallel\omega\,|\,zz')-\lambda\sum_\mu\int\frac{d^2k_\parallel''}{(2\pi)^2}\int dz''\,d_{\lambda\nu}(\vec{k}_\parallel\omega\,|\,zz'')\times\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel'')\,\delta(z'')\,\hat{d}_{\mu\nu}(\vec{k}_\parallel''\vec{k}_\parallel'\omega\,|\,z''z')\ , \tag{2.15}$$

where we have set

$$\lambda=(\omega^2/4\pi c^2)[\epsilon(\omega)-1]\ . \tag{2.16}$$

It might appear that the integration on z'' in Eq. (2.15) should be straightforward to carry out because of the presence of the δ function in the integrand. However, the function $d_{\lambda\mu}(\vec{k}_\parallel\omega|zz'')$ can be discontinuous as a function of z'', across the plane $z''=0$, as can $\hat{d}_{\mu\nu}(\vec{k}_\parallel''\vec{k}_\parallel'\omega|z''z')$. The way in which the integral is to be evaluated, therefore, is not obvious. In earlier work on the scattering and adsorption of electromagnetic waves by surface roughness[8] integrals such as appear in Eq. (2.15) were interpreted according to the rule

$$\int f(z)\,\delta(z)\,g(z)\,dz=\tfrac{1}{2}[f(0+)g(0+)+f(0-)g(0-)]\,, \tag{2.17}$$

in view of the fact that the functions $f(z)$ and $g(z)$ can be discontinuous at $z=0$. However, it was shown subsequently[12,13] that the cross section for the scattering of p-polarized incident radiation into p-polarized scattered radiation obtained in this way is not in agreement with that obtained by the boundary matching method.[13,14] The cross sections for $(s\to s)$, $(s\to p)$, and $(p\to s)$ scattering obtained by the Green's function and boundary matching methods, however, are in agreement.

In his work on the attenuation of surface polaritons Mills[7] pointed out that the results obtained by these two methods can be made to agree completely if Eq. (2.17) is replaced by

$$\int f(z)\,\delta(z)\,g(z)\,dz=f(0+)g(0-)\;. \tag{2.18}$$

Mills did not provide any derivation of this result beyond reference to earlier work by Juranek[15] who showed how effective surface currents might be arranged so as to generate the same scattered fields as are obtained by the boundary matching method. He also demonstrated that when used with the Green's-function method it yields the same result as the boundary matching method. To our knowledge no derivation of the rule (2.18) exists at the present time. We will use it in the present work because it does yield results by the Green's-function method identical with those obtained by the boundary matching method, and because it will make a comparison of our results with those of Mills more meaningful.

With the use of Eq. (2.18) the result of the integration over z'' is given by

$$\begin{aligned}\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|zz')&=(2\pi)^2\,\delta(\vec{k}_\parallel+\vec{k}_\parallel')\,d_{\lambda\nu}(\vec{k}_\parallel\,\omega|zz')\\&\quad-\lambda\sum_\mu d_{\lambda\mu}(\vec{k}_\parallel\omega|z\,0+)\int\frac{d^2k_\parallel''}{(2\pi)^2}\\&\quad\times\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel'')\,\hat{d}_{\mu\lambda}(\vec{k}_\parallel''\vec{k}_\parallel'\omega|0-z').\end{aligned} \tag{2.19}$$

We now set $z=0-$ in this equation to obtain

$$\begin{aligned}\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|0-z')&=(2\pi)^2\delta(\vec{k}_\parallel+\vec{k}_\parallel')\,d_{\lambda\nu}(\vec{k}_\parallel\omega|0-z')\\&-\lambda\sum_\mu d_\mu^{(0)}(\vec{k}_\parallel\omega)\int\frac{d^2k_\parallel''}{(2\pi)^2}\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel'')\,\hat{d}_{\mu\nu}(\vec{k}_\parallel''\vec{k}_\parallel'\omega|0-z')\,,\end{aligned} \tag{2.20}$$

where

$$d_{\lambda\mu}^{(0)}(\vec{k}_\parallel\omega)\equiv d_{\lambda\mu}(\vec{k}_\parallel\omega|0-0+)\;. \tag{2.21}$$

The solution of this equation substituted into Eq. (2.19) yields the desired function $\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|zz')$.

We solve Eq. (2.20) by iteration:

$$\begin{aligned}\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|0-z')&=(2\pi)^2\,\delta(\vec{k}_\parallel+\vec{k}_\parallel')\,d_{\lambda\nu}(\vec{k}_\parallel\omega|0-z')-\lambda\sum_\mu d_{\lambda\mu}^{(0)}(\vec{k}_\parallel\omega)\,\hat{\zeta}(\vec{k}_\parallel+\vec{k}_\parallel')\,d_{\mu\nu}(-\vec{k}_\parallel'\omega|0-z')\\&+\lambda^2\sum_{\mu\mu'}\int\frac{d^2k_\parallel''}{(2\pi)^2}\,d_{\lambda\mu}^{(0)}(\vec{k}_\parallel\omega)\,\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel'')\,d_{\mu\mu'}^{(0)}(\vec{k}_\parallel\omega)\,\zeta(\vec{k}_\parallel''+\vec{k}_\parallel')\,d_{\mu'\nu}(-\vec{k}_\parallel'\omega|0-z')\\&-\lambda^3\sum_{\mu\mu'\mu''}\int\frac{d^2k_\parallel''}{(2\pi)^2}\int\frac{d^2k_\parallel'''}{(2\pi)^2}\,d_{\lambda\mu}^{(0)}(\vec{k}_\parallel\omega)\,\zeta(\vec{k}_\parallel-\vec{k}_\parallel'')\,d_{\mu\mu'}^{(0)}(\vec{k}_\parallel''\omega)\\&\times\hat{\zeta}(\vec{k}_\parallel''-\vec{k}_\parallel''')\,d_{\mu'\mu''}^{(0)}(\vec{k}_\parallel''')\,\hat{\zeta}(\vec{k}_\parallel'''+\vec{k}_\parallel')\,d_{\mu''\nu}(-\vec{k}_\parallel'\omega|0-z')+\cdots\;.\end{aligned} \tag{2.22}$$

In order that we can compare our results with experimental data for a dielectric surface, it is reasonable to assume that the surface profile function $\zeta(\vec{x}_\parallel)$ is a stationary stochastic process, and that the Fourier coefficient $\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|zz')$ obtained by substituting Eq. (2.22) into Eq. (2.19) should be averaged, term by term over the probability distribution function for this process. To carry out this procedure we assume that the Fourier coefficients $\{\hat{\zeta}(\vec{k}_\parallel)\}$ are Gaussianly distributed random variables. This assumption has the consequences that the average of the product of an odd number of $\{\hat{\zeta}(\vec{k}_\parallel)\}$ vanishes, while the average of the product of an even number of these functions is obtained by pairing them two-by-two different in all possible ways and assigning to the average of each pair the value[8]

$$\begin{aligned}\langle\hat{\zeta}(\vec{k}_\parallel)\,\hat{\zeta}(\vec{k}_\parallel')\rangle&=[(2\pi)^2/A]\delta(\vec{k}_\parallel+\vec{k}_\parallel')\langle|\hat{\zeta}(\vec{k}_\parallel)|^2\rangle\\&=\delta(\vec{k}_\parallel+\vec{k}_\parallel')(2\pi)^2\,\delta^2g(k_\parallel)\;.\end{aligned} \tag{2.23}$$

In this result, A is the area of the dielectric surface, δ^2 is the mean-square surface height variation, and the surface scattering factor $g(k_\parallel)$ is assumed to be a function of the magnitude of the vector $\vec{k}_\parallel$, but not of its direction. With the preceding assumptions we have, for example, that

$$\langle\hat{\xi}(\vec{k}_\parallel)\,\hat{\xi}(\vec{k}'_\parallel)\,\hat{\xi}(\vec{k}''_\parallel)\,\hat{\xi}(\vec{k}'''_\parallel)\rangle = \langle\hat{\xi}(\vec{k}_\parallel)\,\hat{\xi}(\vec{k}'_\parallel)\rangle \times\langle\hat{\xi}(k''_\parallel)\,\hat{\xi}(\vec{k}'''_\parallel)\rangle + \langle\hat{\xi}(\vec{k}_\parallel)\,\hat{\xi}(\vec{k}''_\parallel)\rangle\langle\hat{\xi}(\vec{k}'_\parallel)\,\hat{\xi}(\vec{k}'''_\parallel)\rangle + \langle\hat{\xi}(\vec{k}_\parallel)\,\hat{\xi}(\vec{k}'''_\parallel)\rangle\langle\hat{\xi}(\vec{k}'_\parallel)\,\hat{\xi}(\vec{k}''_\parallel)\rangle \; . \qquad (2.24)$$

It follows, therefore, that the quantity of interest in this theory is given by

$$\lambda\int\frac{d^2k_\parallel^{(1)}}{(2\pi)^2}\langle\hat{\xi}(\vec{k}_\parallel-\vec{k}_\parallel^{(1)})\,\hat{d}_{\lambda\nu}(\vec{k}_\parallel^{(1)}\,\vec{k}'_\parallel\,\omega\,|\,0-z')\rangle = -\sum_\mu\Bigg(\lambda^2\int\frac{d^2k_\parallel^{(1)}}{(2\pi)^2}\langle\hat{\xi}(\vec{k}_\parallel-\vec{k}_\parallel^{(1)})\,d_{\lambda\mu}^{(0)}(\vec{k}_\parallel^{(1)}\omega)\,\hat{\xi}(\vec{k}_\parallel^{(1)}+\vec{k}'_\parallel)\rangle$$
$$+\lambda^4\sum_{\mu_1\mu_2}\int\frac{d^2k_\parallel^{(1)}}{(2\pi)^2}\int\frac{d^2k_\parallel^{(2)}}{(2\pi)^2}\int\frac{d^2k_\parallel^{(3)}}{(2\pi)^2}\langle\hat{\xi}(\vec{k}_\parallel-\vec{k}_\parallel^{(1)})\,d_{\lambda\mu_1}^{(0)}(\vec{k}_\parallel^{(1)}\omega)\hat{\xi}(\vec{k}_\parallel^{(1)}-\vec{k}_\parallel^{(2)})\,d_{\mu_1\mu_2}^{(0)}(\vec{k}_\parallel^{(2)}\omega)\hat{\xi}(\vec{k}_\parallel^{(2)}$$
$$-\vec{k}_\parallel^{(3)})d_{\mu_2\mu}^{(0)}(\vec{k}_\parallel^{(3)}\omega)\,\hat{\xi}(\vec{k}_\parallel^{(3)}+\vec{k}'_\parallel)\rangle+\cdots\Bigg)\,d_{\mu\nu}(-\vec{k}'_\parallel\omega\,|\,0-z') \, . \qquad (2.25)$$

When the indicated averages of the products of the $\{\hat{\xi}(\vec{k}_\parallel)\}$ are evaluated according to the prescription given above, the terms in large parentheses in Eq. (2.25) can be represented diagrammatically. In Fig. 1 is given the diagram corresponding to the term of $O(\lambda^2)$ in Eq. (2.25). In Fig. 2 are presented the three diagrams associated with the three ways of pairing the four $\{\hat{\xi}(\vec{k}_\parallel)\}$ in the term of $O(\lambda^4)$ in Eq. (2.25). These three pairing schemes correspond to the three terms on the right-hand side of Eq. (2.24). The heavy horizontal lines labeled by the wave vectors $\vec{k}_\parallel^{(1)}$, $\vec{k}_\parallel^{(2)}, \ldots$, correspond to the (matrix) propagators $d_{\lambda\mu_1}^{(0)}(\vec{k}_\parallel^{(1)}\omega)$, $d_{\mu_1\mu_2}^{(0)}(\vec{k}_\parallel^{(2)}\omega), \ldots$. The light incoming horizontal lines labeled by the wave vectors $\vec{k}_\parallel$ and $-\vec{k}'_\parallel$ correspond to the propagators $d_{\lambda\mu}(\vec{k}_\parallel\omega\,|\,z\,0+)$ and $d_{\mu\nu}(-\vec{k}'_\parallel\omega\,|\,0-z')$, respectively. However, they do not enter the evaluation of the expansion contained in the large parentheses in Eq. (2.25). The dashed lines represent the factors of $\{\hat{\xi}(\vec{k}_\parallel)\}$. The fact that in each diagram the dashed lines are always joined in pairs is a reflection of the fact that owing to our assumption that the $\{\hat{\xi}(\vec{k}_\parallel)\}$ are Gaussianly distributed random variables, the average of a product of an even number of these variables is the sum of products of the averages of these variables paired two-by-two different in all possible ways. From the structure of the expansion in the large parentheses in Eq. (2.25), and the result given by Eq. (2.23), we see that the wave vectors $\{\vec{k}^{(i)}\}$ are conserved at each vertex: the sum of the wave vectors entering each vertex is equal to the sum of the wave vectors leaving it. An immediate consequence of this fact is that the wave vector $-\vec{k}'_\parallel$ is forced to equal the wave vector $\vec{k}_\parallel$, through the presence of a factor $(2\pi)^2\,\delta(\vec{k}_\parallel+\vec{k}'_\parallel)$ in each term. Thus the averaging of the Green's function $\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}'_\parallel\omega\,|\,zz')$ over the probability distribution function for the surface profile function restores infinitesimal translational invariance to our system in the directions parallel to the surface of the dielectric medium.

In addition, we see that this averaging process forces some of the integration variables $\{\vec{k}_\parallel^{(1)}\}$ appearing in the expansion in large parentheses in Eq. (2.25) to equal the wave vector $\vec{k}_\parallel$.

A typical diagram contributing to the expansion in large parentheses in Eq. (2.25) thus has the following structure. A line $(\vec{k}_\parallel)$ enters the diagram at the left, interactions of all degrees of complexity occur, and a line $(\vec{k}_\parallel)$ leaves the diagram at the right. From Figs. 1 and 2 we see that these diagrams fall into two types: those that can be separated into two unconnected parts by cutting a single heavy line; and those that cannot. The former type of a diagram is called "improper"; the latter type is called "proper." Examples of proper diagrams are Figs. 1, 2(b), and 2(c), whereas Fig. 2(a) depicts an improper diagram. It should be noted that because of the conservation of wave vectors at each vertex, any heavy line in an improper diagram which can be cut to separate it into two unconnected parts must be labeled by the wave vector $\vec{k}_\parallel$.

The expansion in large parentheses in Eq. (2.25) can be expressed in terms of contributions from proper diagrams only. We introduce a matrix $\mathcal{P}_{\lambda\mu}(\vec{k}_\parallel\,\omega)$ that is defined as the sum of the contributions in the expansion in large parentheses in Eq. (2.25) associated with the proper diagrams only, excluding the factor $(2\pi)^2\,\delta(\vec{k}_\parallel+\vec{k}'_\parallel)$, which is common to each term. In terms of this matrix we obtain

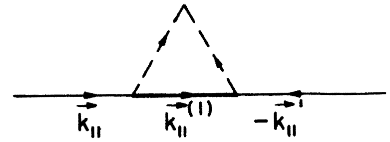

FIG. 1. Diagram corresponding to the term of $O(\lambda^2)$ in Eq. (2.25).

$$\lambda \int \frac{d^2k_\parallel^{(1)}}{(2\pi)^2} \langle \hat{\xi}(\vec{k}_\parallel - \vec{k}_\parallel^{(1)})\, \hat{d}_{\lambda\nu}(\vec{k}_\parallel^{(1)} \vec{k}_\parallel' \omega \,|\, 0 - z')\rangle$$

$$= -(2\pi)^2\, \delta(\vec{k}_\parallel + \vec{k}_\parallel') \sum_{\mu} \Big(\mathcal{P}_{\lambda\mu}(\vec{k}_\parallel \omega) + \sum_{\mu_1\mu_2} \mathcal{P}_{\lambda\mu_1}(\vec{k}_\parallel \omega)\, d^{(0)}_{\mu_1\mu_2}(\vec{k}_\parallel \omega)\, \mathcal{P}_{\mu_2\mu}(\vec{k}_\parallel \omega) + \ldots \Big) d_{\mu\nu}(\vec{k}_\parallel \omega \,|\, 0 - z')$$

$$= -(2\pi)^2\, \delta(\vec{k}_\parallel + \vec{k}_\parallel') \sum_{\mu} [\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega) + \overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega)\, \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega)\, \overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega) + \cdots]_{\lambda\mu}\, d_{\mu\nu}(\vec{k}_\parallel \omega \,|\, 0 - z')$$

$$= -(2\pi)^2\, \delta(\vec{k}_\parallel + \vec{k}_\parallel') \sum_{\mu} [\overleftrightarrow{\mathcal{P}}^{-1}(\vec{k}_\parallel \omega) - \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega)]^{-1}_{\lambda\mu}\, d_{\mu\nu}(\vec{k}_\parallel \omega \,|\, 0 - z') \; . \tag{2.26}$$

When we substitute this result into Eq. (2.19), we obtain finally for the averaged Fourier coefficient of the desired Green's function

$$\langle \hat{d}_{\lambda\nu}(\vec{k}_\parallel \vec{k}_\parallel' \omega \,|\, zz')\rangle = (2\pi)^2 \delta(\vec{k}_\parallel + \vec{k}_\parallel') \Big(d_{\mu\nu}(\vec{k}_\parallel \omega \,|\, zz') + \sum_{\mu_1\mu_2} d_{\lambda\mu_1}(\vec{k}_\parallel \omega \,|\, z\, 0+) [\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega)^{-1} - \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega)]^{-1}_{\mu_1\mu_2} \times d_{\mu_2\nu}(\vec{k}_\parallel \omega \,|\, 0 - z') \Big). \tag{2.27}$$

In the lowest order of approximation $O(\delta^2)$, which is all that is justified because we have kept only terms of first order in $\zeta(\vec{x}_\parallel)$ in Eq. (2.9), the elements of the matrix $\mathcal{P}_{\mu\nu}(\vec{k}_\parallel \omega)$ are given by

$$\mathcal{P}_{\mu\nu}(\vec{k}_\parallel \omega) = \lambda^2 \delta^2 \int \frac{d^2k_\parallel'}{(2\pi)^2}\, g(|\vec{k}_\parallel - \vec{k}_\parallel'|)\, d^{(0)}_{\mu\nu}(\vec{k}_\parallel' \omega) \; . \tag{2.28}$$

Equations (2.27) and (2.28) are the central results of this section. They provide the basis for a calculation of the cross section for the Raman scattering of light from a semi-infinite dielectric medium bounded by a rough surface. We will not pursue this application here. Instead, we will determine the poles $\omega(\vec{k}_\parallel)$ of $\langle \hat{d}_{\lambda\nu}(\vec{k}_\parallel \vec{k}_\parallel' \omega \,|\, zz')\rangle$ corresponding to surface polaritons, and in this way determine the attenuation of surface polaritons owing to surface roughness.

III. DISPERSION RELATION FOR SURFACE POLARITONS

In this section we obtain the inverse matrix $[\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega)^{-1} - \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega)]^{-1}$ and study its poles. This is because the matrix elements $d_{\lambda\nu}(\vec{k}_\parallel \omega \,|\, zz')$ have a pole at the frequency $\omega_0(k_\parallel)$ of a surface polariton associated with a plane surface separating the dielectric medium from the vacuum.[8] Thus the poles of the function $\langle \hat{d}_{\lambda\nu}(\vec{k}_\parallel \vec{k}_\parallel' \omega \,|\, zz')\rangle$ corresponding to the frequencies of surface polaritons shifted by the presence of surface roughness can only come from the poles of the matrix $[\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega)^{-1} - \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega)]^{-1}$.

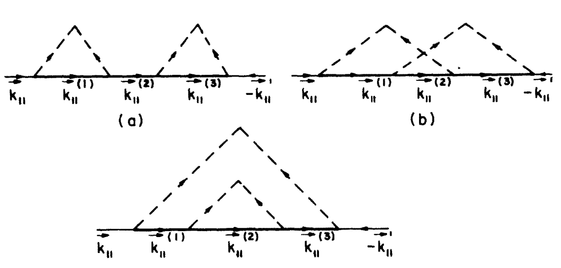

FIG. 2. Three diagrams corresponding to the terms of $O(\lambda^4)$ in Eq. (2.25).

It has been shown[8] that the functions $d_{\mu\nu}(\vec{k}_\parallel \omega | zz')$ are expressible in terms of simpler functions $g_{\mu\nu}(k_\parallel \omega | zz')$ according to

$$d_{\mu\nu}(\vec{k}_\parallel \omega \,|\, zz') = \sum_{\mu'\nu'} S^{-1}_{\mu\mu'}(\hat{k}_\parallel)\, g_{\mu'\nu'}(k_\parallel \omega \,|\, zz') S_{\nu'\nu}(\hat{k}_\parallel) \; , \tag{3.1}$$

where the matrix $\overleftrightarrow{S}(\hat{k}_\parallel)$ is given by

$$\overleftrightarrow{S}(\hat{k}_\parallel) = \begin{pmatrix} \hat{k}_x & \hat{k}_y & 0 \\ -\hat{k}_y & \hat{k}_x & 0 \\ 0 & 0 & 1 \end{pmatrix} ,$$

$$\overleftrightarrow{S}(\hat{k}_\parallel)^{-1} = \begin{pmatrix} \hat{k}_x & -\hat{k}_y & 0 \\ \hat{k}_y & \hat{k}_x & 0 \\ 0 & 0 & 1 \end{pmatrix} , \tag{3.2}$$

with $\hat{k}_\alpha = k_\alpha / k_\parallel$ $(\alpha = x, y)$. Note that $g_{\mu\nu}(k_\parallel \omega | zz')$ depends on $\vec{k}_\parallel$ only through its magnitude. Thus, if we define a matrix

$$\overleftrightarrow{M}(\vec{k}_\parallel \omega) = \overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega)^{-1} - \overleftrightarrow{d}^{(0)}(\vec{k}_\parallel \omega) \; , \tag{3.3}$$

and use Eq. (3.1), we can write

$$\overleftrightarrow{M}(\vec{k}_\parallel \omega)^{-1} = \overleftrightarrow{S}(\hat{k}_\parallel)^{-1} \{[\overleftrightarrow{S}(\hat{k}_\parallel) \overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel \omega) \overleftrightarrow{S}(\hat{k}_\parallel)^{-1}]^{-1} - \overleftrightarrow{g}^{(0)}(k_\parallel \omega)\}^{-1} \overleftrightarrow{S}(\hat{k}_\parallel) \; , \tag{3.4}$$

where

$$g^{(0)}_{\mu\nu}(k_\parallel \omega) \equiv g_{\mu\nu}(k_\parallel \omega \,|\, 0 - 0+) \; . \tag{3.5}$$

The functions $\{g_{\mu\nu}(k_\parallel \omega | zz')\}$ are tabulated in Ref. 8. From the results of Ref. 8 we find that the matrix $\overleftrightarrow{g}^{(0)}(k_\parallel \omega)$ has the simple form

$$g^{(0)}(k_{\parallel}\omega)=\frac{4\pi i c^2}{\omega^2}\begin{pmatrix}\dfrac{-kk_1}{k_1-\epsilon(\omega)k} & 0 & \dfrac{-k_{\parallel}k_1}{k_1-\epsilon(\omega)k}\\ 0 & \dfrac{\omega^2}{c^2}\dfrac{1}{k_1-k} & 0\\ \dfrac{k_{\parallel}k}{k_1-\epsilon(\omega)k} & 0 & \dfrac{k_{\parallel}^2}{k_1-\epsilon(\omega)k}\end{pmatrix}\equiv\frac{4\pi i c^2}{\omega^2}\overleftrightarrow{\gamma}^{(0)}(k_{\parallel}\omega)\ , \tag{3.6}$$

where

$$k=\begin{cases}(\omega^2/c^2-k_{\parallel}^2)^{1/2}\ , & k_{\parallel}<\omega/c\ ,\\ i(k_{\parallel}^2-\omega^2/c^2)^{1/2}\ , & k_{\parallel}>\omega/c\ ,\end{cases} \tag{3.7}$$

$$k_1=-[\epsilon(\omega)(\omega^2/c^2)-k_{\parallel}^2]^{1/2}\ ,\quad \mathrm{Im}k_1<0\ . \tag{3.8}$$

In writing Eq. (3.8) we have used the fact that $\mathrm{Im}\epsilon(\omega)>0$.

For the surface scattering factor we assume the Gaussian form

$$g(k_{\parallel})=\pi a^2 e^{-a^2k_{\parallel}^2/4}\ , \tag{3.9}$$

where the constant a is called the transverse correlation length. When we substitute this expression into Eq. (2.26), and make use of Eqs. (3.1), (3.5), and (3.6), we find that the matrix $\mathcal{P}_{\mu\nu}(\vec{k}_{\parallel}\omega)$ takes the form

$$\overleftrightarrow{\mathcal{P}}(\vec{k}_{\parallel}\omega)=i\frac{\lambda^2\delta^2a^2c^2}{\omega^2}e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\int_0^{2\pi}d\theta'\,e^{a^2k_{\parallel}k_{\parallel}'\cos(\theta-\theta')/2}$$
$$\times\begin{pmatrix}\gamma_{xx}'\cos^2\theta'+\gamma_{yy}'\sin^2\theta' & (\gamma_{xx}'-\gamma_{yy}')\cos\theta'\sin\theta' & \gamma_{xz}'\cos\theta'\\ (\gamma_{xx}'-\gamma_{yy}')\cos\theta'\sin\theta' & \gamma_{xx}'\sin^2\theta'+\gamma_{yy}'\cos^2\theta' & \gamma_{xz}'\sin\theta'\\ \gamma_{zx}'\cos\theta' & \gamma_{zx}'\sin\theta' & \gamma_{zz}'\end{pmatrix}, \tag{3.10}$$

where, to simplify the notation, we have written $\gamma_{\mu\nu}'\equiv\gamma_{\mu\nu}^{(0)}(k_{\parallel}'\omega)$. In addition, we have set

$$\vec{k}_{\parallel}=k_{\parallel}(\cos\theta,\ \sin\theta),\quad \vec{k}_{\parallel}'=k_{\parallel}'(\cos\theta',\ \sin\theta')\ . \tag{3.11}$$

The integrals over θ' are carried out directly, with the result that

$$\overleftrightarrow{\mathcal{P}}(\vec{k}_{\parallel}\omega)=2\pi i\frac{\lambda^2\delta^2a^2c^2}{\omega^2}\begin{pmatrix}-\frac{1}{2}[a+b(\hat{k}_x^2-\hat{k}_y^2)] & -b\hat{k}_x\hat{k}_y & -d\hat{k}_x\\ -b\hat{k}_x\hat{k}_y & -\frac{1}{2}[a-b(\hat{k}_x^2-\hat{k}_y^2)] & -d\hat{k}_y\\ c\hat{k}_x & c\hat{k}_y & e\end{pmatrix}, \tag{3.12}$$

where

$$a(k_{\parallel}\omega)=e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\times\left(\frac{k'k_1'}{k_1'-\epsilon(\omega)k'}-\frac{\omega^2}{c^2}\frac{1}{k_1'-k'}\right)I_0(\tfrac{1}{2}a^2k_{\parallel}k_{\parallel}')\ , \tag{3.13a}$$

$$b(k_{\parallel}\omega)=e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\times\left(\frac{k'k_1'}{k_1'-\epsilon(\omega)k'}+\frac{\omega^2}{c^2}\frac{1}{k_1'-k'}\right)I_2(\tfrac{1}{2}a^2k_{\parallel}k_{\parallel}')\ , \tag{3.13b}$$

$$c(k_{\parallel}\omega)=e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\times\frac{k_{\parallel}'k'}{k_1'-\epsilon(\omega)k'}I_1(\tfrac{1}{2}a^2k_{\parallel}k_{\parallel}')\ , \tag{3.13c}$$

$$d(k_{\parallel}\omega)=e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\times\frac{k_{\parallel}'k_1'}{k_1'-\epsilon(\omega)k'}I_1(\tfrac{1}{2}a^2k_{\parallel}k_{\parallel}')\ , \tag{3.13d}$$

$$e(k_{\parallel}\omega)=e^{-a^2k_{\parallel}^2/4}\int_0^{\infty}dk_{\parallel}'k_{\parallel}'e^{-a^2k_{\parallel}'^2/4}\times\frac{k_{\parallel}'^2}{k_1'-\epsilon(\omega)k'}I_0(\tfrac{1}{2}a^2k_{\parallel}k_{\parallel}')\ , \tag{3.13e}$$

where $k'=k(k_{\parallel}')$ and $k_1'=k_1(k_{\parallel}')$, and $I_n(x)$ is the modified Bessel function of the first kind.

It follows from Eq. (3.12) that

$$\overleftrightarrow{S}(\hat{k}_\parallel)\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel\omega)\overleftrightarrow{S}(\vec{k}_\parallel)^{-1}=2\pi i\,\frac{\lambda^2\delta^2a^2c^2}{\omega^2}\begin{pmatrix}-\frac{1}{2}(a+b) & 0 & -d\\ 0 & -\frac{1}{2}(a-b) & 0\\ c & 0 & e\end{pmatrix}. \tag{3.14}$$

The inversion of this matrix is straightforward, and yields the result

$$[\overleftrightarrow{S}(\hat{k}_\parallel)\overleftrightarrow{\mathcal{P}}(\vec{k}_\parallel\omega)\overleftrightarrow{S}(\hat{k}_\parallel)^{-1}]^{-1}=\frac{\omega^2}{2\pi i\lambda^2\delta^2a^2c^2}\begin{pmatrix}\frac{-2e}{(a+b)e-2dc} & 0 & \frac{-2d}{(a+b)e-2dc}\\ 0 & \frac{-2}{a-b} & 0\\ \frac{2c}{(a+b)e-2dc} & 0 & \frac{a+b}{(a+b)e-2dc}\end{pmatrix}\equiv\frac{\omega^2}{2\pi i\lambda^2\delta^2a^2c^2}\overleftrightarrow{p}(k_\parallel\omega)\,. \tag{3.15}$$

Consequently, the matrix $\overleftrightarrow{M}(\hat{k}_\parallel\omega)^{-1}$ which we seek is given by

$$\overleftrightarrow{M}(\vec{k}_\parallel\omega)^{-1}=-\frac{\omega^2}{4\pi i c^2}\overleftrightarrow{S}(\hat{k}_\parallel)^{-1}\left(\overleftrightarrow{\gamma}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}\overleftrightarrow{p}(k_\parallel\omega)\right)^{-1}\overleftrightarrow{S}(\hat{k}_\parallel)$$

$$=-\frac{\omega^2}{4\pi i c^2}\overleftrightarrow{S}(\hat{k}_\parallel)^{-1}\overleftrightarrow{m}(k_\parallel\omega)\overleftrightarrow{S}(\hat{k}_\parallel)\,. \tag{3.16}$$

The elements of the matrix $\overleftrightarrow{m}(k_\parallel\omega)$ are readily obtained, and the nonzero elements are given by

$$m_{xx}(k_\parallel\omega)=\frac{1}{D(k_\parallel\omega)}\left(\gamma_{zz}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}p_{zz}(k_\parallel\omega)\right), \tag{3.17a}$$

$$m_{xz}(k_\parallel\omega)=\frac{-1}{D(k_\parallel\omega)}\left(\lambda_{xz}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}p_{xz}(k_\parallel\omega)\right), \tag{3.17b}$$

$$m_{zx}(k_\parallel\omega)=\frac{-1}{D(k_\parallel\omega)}\left(\gamma_{zx}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}p_{zx}(k_\parallel\omega)\right), \tag{3.17c}$$

$$m_{zz}(k_\parallel\omega)=\frac{1}{D(k_\parallel\omega)}\left(\gamma_{xx}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}p_{xx}(k_\parallel\omega)\right), \tag{3.17d}$$

$$m_{yy}(k_\parallel\omega)=\left(\gamma_{yy}^{(0)}(k_\parallel\omega)+\frac{1}{8\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}p_{yy}(k_\parallel\omega)\right)^{-1}, \tag{3.17e}$$

where

$$D(k_\parallel\omega)=\frac{1}{8\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}\frac{1}{(a+b)e-2dc}\left(\frac{1}{k_1-\epsilon(\omega)k}\times[-2k_\parallel^2e-kk_1(a+b)+2k_\parallel kd+2k_\parallel k_1c]-\frac{1}{4\pi^2\lambda^2\delta^2a^2}\frac{\omega^4}{c^4}\right). \tag{3.18}$$

Just as the Green's functions $\{d_{\mu\nu}(\vec{k}_\parallel\omega|zz')\}$ can be expressed in terms of the simpler functions $\{g_{\mu\nu}(k_\parallel\omega|zz')\}$, according to Eq. (3.1), the Green's functions $\langle\hat{d}_{\lambda\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|zz')\rangle$ can also be expressed in terms of simpler functions. If we make use of Eq. (2.25) and Eqs. (3.1), (3.4), and (3.16), we find that

$$\langle d_{\mu\nu}(\vec{k}_\parallel\vec{k}_\parallel'\omega|zz')\rangle=(2\pi)^2\delta(\vec{k}_\parallel+\vec{k}_\parallel')\sum_{\mu'\nu'}S_{\mu\mu'}^{-1}(\hat{k}_\parallel)\times\hat{g}_{\mu'\nu'}(k_\parallel\omega|zz')S_{\nu'\nu}(\hat{k}_\parallel)\,, \tag{3.19}$$

where

$$\hat{g}_{\mu\nu}(k_\parallel\omega|zz')=g_{\mu\nu}(k_\parallel\omega|zz')-\frac{\omega^2}{4\pi i c^2}\times\sum_{\mu'\nu'}g_{\mu\mu'}(k_\parallel\omega|z\,0+)\,m_{\mu'\nu'}(k_\parallel\omega)\,g_{\nu'\nu}(k_\parallel\omega|0-z')\,. \tag{3.20}$$

In searching for the pole of the matrix $\overleftrightarrow{m}(k_\parallel\omega)$, which in the absence of surface roughness reduces to the dispersion relation for surface polaritons associated with a plane dielectric-vacuum interface, we note the identity

$$\frac{1}{k_1-\epsilon(\omega)k}=-\frac{c^2}{\omega^2}\frac{k_1+\epsilon(\omega)k}{1-\epsilon^2(\omega)}\frac{1}{c^2k_\parallel^2/\omega^2-\epsilon(\omega)/[\epsilon(\omega)+1]}, \tag{3.21}$$

and recall that the solution of the equation

$$c^2k_\parallel^2/\omega^2=\epsilon(\omega)/[\epsilon(\omega)+1] \tag{3.22}$$

is the dispersion relation $\omega=\omega_0(k_\parallel)$ for surface polaritons at a plane dielectric-vacuum interface.[2] Thus the function $k_1-\epsilon(\omega)k$ has a simple zero at $\omega=\omega_0(k_\parallel)$. It follows then [from Eqs. (3.17) and (3.18)] that the pole of the matrix $\overleftrightarrow{m}(k_\parallel\omega)$ corresponding to a rough surface polariton is given by the zero of the function $D(k_\parallel\omega)$. From Eq. (3.18) we see that the equation $D(k_\parallel\,\omega)=0$ can be written equivalently as

$$k_1 - \epsilon(\omega)k = 4\pi^2\lambda^2\delta^2 a^2(c^4/\omega^4)G(k_\parallel\omega) , \tag{3.23}$$

where

$$G(k_\parallel\omega) = -2k_\parallel^2 e(k_\parallel\omega) - kk_1[a(k_\parallel\omega) + b(k_\parallel\omega)] + 2k_\parallel[kd(k_\parallel\omega) + k_1 c(k_\parallel\omega)] . \tag{3.24}$$

If we define

$$F(k_\parallel\omega) = k_1 - \epsilon(\omega)k , \tag{3.25}$$

and denote by $\omega_0(k_\parallel)$ the solution of $F(k_\parallel\omega) = 0$, the solution of Eq. (3.23) correct to $O(\delta^2)$ is given by

$$\omega(k_\parallel) = \omega_0(k_\parallel) + \tfrac{1}{4}\delta^2 a^2\left(\frac{G(k_\parallel\omega)}{(d/d\omega)F(k_\parallel\omega)}\right)_{\omega=\omega_0(k_\parallel)} . \tag{3.26}$$

Equation (3.26), together with Eqs. (3.24), (3.25), (3.7)–(3.18), and (3.13), formally solves the problem of obtaining the surface roughness induced shift in the surface polariton dispersion relation. In Sec. IV we turn to the evaluation of the second term on the right-hand side of Eq. (3.26) for several cases of physical interest.

IV. NUMERICAL RESULTS

In this section we utilize the results of Sec. III to obtain numerical results for the surface polariton dispersion curve in the presence of surface roughness through terms of $O(\delta^2)$. In these calculations we will utilize two different forms for the dielectric constant $\epsilon(\omega)$. The first of these,

$$\epsilon(\omega) = \epsilon_\infty + \frac{(\epsilon_0 - \epsilon_\infty)\omega_T^2}{\omega_T^2 - \omega^2 - i\omega\gamma} , \tag{4.1}$$

corresponds to the case of a diatomic, cubic polar crystal with two ions in a primitive unit cell; the second,

$$\epsilon(\omega) = \epsilon_\infty[1 - \omega_p^2/(\omega^2 + i\omega\gamma)] , \tag{4.2}$$

represents the contribution to the dielectric constant of a nearly-free-electron metal or n-type semiconductor from intraband transitions. In Eq. (4.1) ϵ_∞ is the optical frequency dielectric constant, ϵ_0 is the static dielectric constant, and ω_T is the frequency of the infinite wavelength transverse optical vibration modes. In Eq. (4.2) ϵ_∞ is the background dielectric constant of the material, and ω_p is the electronic plasma frequency, given by

$$\omega_p^2 = \frac{4\pi n e^2}{m^* \epsilon_\infty} , \tag{4.3}$$

where n is the electron number density, e is the magnitude of the electronic charge, and m^* is the effective mass of the charge carriers. In both Eqs. (4.1) and (4.2) the damping constant γ describes in a phenomenological way the effects on the dielectric constant of the dissipative processes present in the bulk of the material.

In the case of a polariton propagating along a perfectly smooth surface, an expression for its attenuation length can be obtained by inserting the complex dielectric constant of the material into the equation [Eq. (3.22)] relating the frequency of the surface polariton to the magnitude of its wave vector, and obtaining from it the imaginary part of the wave vector of the surface polariton $k_\parallel^{(I)}$. The attenuation length for energy flow is then $(2k_\parallel^{(I)})^{-1}$.

However, in the presence of surface roughness a surface polariton can be attenuated even if the dielectric constant $\epsilon(\omega)$ is real. It is this effect on which we have focused attention in this paper. Therefore to separate the attenuation of surface polaritons which has its origin in the surface roughness from that which has its origin in the dissipative processes present in the bulk of the material, we will put $\gamma = 0$ in the expressions for the dielectric constants given by Eqs. (4.1) and (4.2) everywhere except in the integrands of the integrals for the functions $a(k_\parallel\omega), \ldots, e(k_\parallel\omega)$ defined by Eqs. (3.13) in evaluating the expressions given at the end of Sec. III. The retention of the (small) imaginary part of the dielectric constant in these integrands serves only to define the manner in which the pole in the integrand at the wave vector of the plane interface surface polariton, i.e., at the value of $k_\parallel'$ for which $k_1' - \epsilon(\omega)k'$ vanishes, is to be treated in the evaluation of these integrals.

When this is done the frequency $\omega_0(k_\parallel)$ of a surface polariton at a plane dielectric-vacuum interface is purely real. It is in fact given by

$$\omega_0^2(k_\parallel) = \frac{1}{2}\left(\frac{c^2k_\parallel^2}{\epsilon_\infty}(1+\epsilon_\infty) + \omega_L^2\right) - \frac{1}{2}\left[\left(\frac{c^2k_\parallel^2}{\epsilon_\infty}(1+\epsilon_\infty) + \omega_L^2\right)^2 - 4\frac{c^2k_\parallel^2}{\epsilon_\infty}(\omega_T^2 + \epsilon_\infty\omega_L^2)\right]^{1/2} , \tag{4.4}$$

where $\omega_L^2 = (\epsilon_0/\epsilon_\infty)\omega_T^2$ for the dielectric constant given by Eq. (4.1), and by

$$\omega_0^2(k_\parallel) = \frac{1}{2}\left(\frac{c^2k_\parallel^2}{\epsilon_\infty}(1+\epsilon_\infty) + \omega_p^2\right) - \frac{1}{2}\left[\left(\frac{c^2k_\parallel^2}{\epsilon_\infty}(1+\epsilon_\infty) + \omega_p^2\right)^2 - 4c^2k_\parallel^2\omega_p^2\right]^{1/2} \tag{4.5}$$

for the dielectric constant given by Eq. (4.2).

Consequently, we can write the dispersion relation (3.26) in the form

$$\omega(k_\parallel) = \omega_0(k_\parallel) + \Delta(k_\parallel) - i\Gamma(k_\parallel) , \tag{4.6}$$

where $\Delta(k_\parallel)$ gives the shift in the frequency of the surface polariton due to surface roughness, while $\Gamma(k_\parallel)$ is related to the inverse lifetime of this mode owing to surface roughness. These two quantities are given by

$$\Delta(k_\parallel)=\tfrac{1}{4}(\delta a)^2[\epsilon(\omega_0)-1]^2\,\mathrm{Re}\left(\frac{G(k_\parallel\omega_0)}{(d/d\omega_0)F(k_\parallel\omega_0)}\right) \quad (4.7)$$

$$\Gamma(k_\parallel)=-\tfrac{1}{4}(\delta a)^2[\epsilon(\omega_0)-1]^2\,\mathrm{Im}\left(\frac{G(k_\parallel\omega_0)}{(d/d\omega_0)F(k_\parallel\omega_0)}\right), \quad (4.8)$$

where, to simplify notation, we have written $\omega_0=\omega_0(k_\parallel)$.

The quantity $\Gamma(k_\parallel)$ is the inverse of the lifetime for the amplitude of the electric field of the surface polariton. Since the energy transported by the surface polariton is proportional to the square of this amplitude, the inverse of the lifetime of the surface polariton $\tau(k_\parallel)$ is given by $2\Gamma(k_\parallel)$,

$$1/\tau(k_\parallel)=2\Gamma(k_\parallel)\ . \quad (4.9)$$

The attenuation length of the surface polariton $l(k_\parallel)$, which is the distance over which the energy in the polariton decays to $1/e$ of its initial value, is obtained by multiplying its lifetime by the energy transport velocity of the surface polariton, $V_E(k_\parallel)$:

$$l(k_\parallel)=V_E(k_\parallel)\,\tau(k_\parallel)=\tfrac{1}{2}[V_E(k_\parallel)/\Gamma(k_\parallel)]\ . \quad (4.10)$$

In the absence of damping the energy transport velocity is equal to the group velocity of the surface polariton.[3] The latter can be obtained most directly by differentiation with respect to ω of the dispersion relation [Eq. (3.22)]. The result is

$$V_E(k_\parallel)=\left(\frac{\partial\omega}{\partial k_\parallel}\right)_{\omega_0}=\frac{e^2k_\parallel}{\omega_0}\times\frac{[\epsilon(\omega_0)+1]^2}{\epsilon(\omega_0)[\epsilon(\omega_0)+1]+\frac{1}{2}\omega_0[d\epsilon(\omega_0)/d\omega_0]}\ . \quad (4.11)$$

We can further simplify the expression for the attenuation length by considering more carefully the derivative with respect to frequency of the function $F(k_\parallel\omega)$, defined by Eqs. (3.7), (3.8), and (3.25), which appears in the definitions of $\Delta(k_\parallel)$ and $\Gamma(k_\parallel)$. For the evaluation of this quantity we note that in the surface polariton regime $k_\parallel>\omega/c$, and $\epsilon(\omega)<0$.[2] Thus, according to Eqs. (3.7) and (3.8) in this regime

$$k=i(k_\parallel^2-\omega^2/c^2)^{1/2},\quad k_1=-i[k_\parallel^2-\epsilon(\omega)(\omega^2/c^2)]^{1/2}\ . \quad (4.12)$$

Therefore it follows that

$$\frac{dF(k_\parallel\omega_0)}{d\omega_0}=-\frac{i}{c}\,\frac{|\epsilon(\omega_0)|+1}{|\epsilon(\omega_0)|[|\epsilon(\omega_0)|-1]^{1/2}}\times\left(\epsilon(\omega_0)[\epsilon(\omega_0)+1]+\frac{\omega_0}{2}\,\frac{d\epsilon(\omega_0)}{d\omega_0}\right)$$
$$=-i\,\frac{ck_\parallel}{\omega_0}\,\frac{[|\epsilon(\omega_0)|+1][|\epsilon(\omega_0)|-1]^{3/2}}{|\epsilon(\omega_0)|}\,\frac{1}{V_E(k_\parallel)}\ . \quad (4.13)$$

Consequently, if we separate the quantity $G(k_\parallel\omega_0)$ into its real and imaginary parts according to

$$G(k_\parallel\omega_0)=G^{(1)}(k_\parallel\omega_0)+iG^{(2)}(k_\parallel\omega_0)\ , \quad (4.14)$$

then on combining Eqs. (4.7) and (4.8) with Eqs. (4.13) and (4.14) we obtain

$$\Delta(k_\parallel)=-\frac{\omega_0}{4ck_\parallel}(\delta a)^2\,\frac{|\epsilon(\omega_0)|[|\epsilon(\omega_0)|+1]}{[|\epsilon(\omega_0)|-1]^{3/2}}\times V_E(k_\parallel)\,G^{(2)}(k_\parallel\omega_0)\ , \quad (4.15)$$

$$\Gamma(k_\parallel)=-\frac{\omega_0}{4ck_\parallel}(\delta a)^2\,\frac{|\epsilon(\omega_0)|[|\epsilon(\omega_0)|+1]}{[|\epsilon(\omega_0)|-1]^{3/2}}\times V_E(k_\parallel)\,G^{(1)}(k_\parallel\omega_0)\ . \quad (4.16)$$

Finally, from Eqs. (4.10) and (4.16) we obtain for the inverse attenuation length of a surface polariton owing to surface roughness

$$\frac{1}{l(k_\parallel)}=-\frac{\omega_0}{2ck_\parallel}(\delta a)^2\,\frac{|\epsilon(\omega_0)|[|\epsilon(\omega_0)|+1]}{[|\epsilon(\omega_0)|-1]^{3/2}}\times G^{(1)}(k_\parallel\omega_0)\ . \quad (4.17)$$

We have carried out numerical calculations of $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, and $l^{-1}(k_\parallel)$ as functions of $k_\parallel$ for both forms of the dielectric constant $\epsilon(\omega)$ given by Eqs. (4.1) and (4.2). Inasmuch as $\omega_0(k_\parallel)$, $\epsilon(\omega_0(k_\parallel))$, and $V_E(k_\parallel)$ are calculated straightforwardly from Eqs. (4.4) and (4.5), (4.1) and (4.2), and (4.11), respectively, it is necessary to discuss only the evaluation of the functions $G^{(1)}(k_\parallel\omega_0)$ and $G^{(2)}(k_\parallel\omega_0)$ in any detail.

We begin by formally separating each of the five functions $a(k_\parallel\omega),\ldots,e(k_\parallel\omega)$ into their real and imaginary parts according to

$$a(k_\parallel\omega)=a^{(1)}(k_\parallel\omega)+ia^{(2)}(k_\parallel\omega),\ldots,\ e(k_\parallel\omega)=e^{(1)}(k_\parallel\omega)+ie^{(2)}(k_\parallel\omega)\ .$$

We also recall that in the surface polariton regime $k_\parallel>\omega/c$, and $\epsilon(\omega)<0$, so that in this regime k and k_1 are pure imaginary and are given by Eqs. (4.12), which we rewrite as

$$k=i(k_\parallel^2-\omega^2/c^2)^{1/2}\equiv i\hat{k}_\beta \quad (4.18\text{a})$$

$$k_1=-i[k_\parallel^2-\epsilon(\omega)(\omega^2/c^2)]^{1/2}\equiv-i\hat{k}_1\ , \quad (4.18\text{b})$$

where $\hat{k}_\beta$ and $\hat{k}_1$ are real. We can thus write for the real and imaginary parts of $G(k_\parallel\omega)$ in this regime

$$G^{(1)}(k_\parallel\omega)=-2k_\parallel^2e^{(1)}(k_\parallel\omega)-\hat{k}_\beta\hat{k}_1[a^{(1)}(k_\parallel\omega)+b^{(1)}(k_\parallel\omega)]+2k_\parallel[-\hat{k}_\beta d^{(2)}(k_\parallel\omega)+\hat{k}_1c^{(2)}(k_\parallel\omega)]\ , \quad (4.19\text{a})$$

$$G^{(2)}(k_\parallel\omega)=-2k_\parallel^2e^{(2)}(k_\parallel\omega)-\hat{k}_\beta\hat{k}_1[a^{(2)}(k_\parallel\omega)+b^{(2)}(k_\parallel\omega)]+2k_\parallel[\hat{k}_\beta d^{(1)}(k_\parallel\omega)-\hat{k}_1c^{(1)}(k_\parallel\omega)]\ . \quad (4.19\text{b})$$

We now turn to the determination of $a^{(1,2)}(k_\parallel\omega),\ldots,e^{(1,2)}(k_\parallel\omega)$.

We first divide the integration over $k_\parallel'$ in Eqs. (3.13) into two integrals, the first over the interval $(0, \omega/c)$ and the second over the interval $(\omega/c, \infty)$. We do this because the nature of the integrand is different in the two intervals. However, this separation also has a physical significance. The wave-vector interval $0 \le k_\parallel' < \omega/c$ is that in which the solutions of Maxwell's equations are propagating, wavelike modes. The interval $k_\parallel' > \omega/c$ is that in which surface polaritons can exist. Thus the contributions to the integrals $a^{(1,2)}(k_\parallel\omega), \ldots, e^{(1,2)}(k_\parallel\omega)$ from these two intervals yield the contributions to $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, and $l^{-1}(k_\parallel)$ from roughness induced scattering of a surface polariton into radiating modes in the vacuum and into other surface polariton modes, respectively.

In obtaining the contribution to each of these integrals from the intervals $0 \le k_\parallel' < \omega/c$ and $\omega/c < k_\parallel'$, it is convenient to define, in analogy with Eqs. (4.18),

$$k_1' = -i[k_\parallel'^2 - \epsilon(\omega)(\omega^2/c^2)]^{1/2} \equiv -i\hat{k}_1' \,, \tag{4.20a}$$

$$k' = \begin{cases} (\omega^2/c^2 - k_\parallel'^2)^{1/2} \equiv \hat{k}_\alpha', & 0 \le k_\parallel' < \omega/c \,, \quad (4.20\text{b}) \\ i(k_\parallel'^2 - \omega^2/c^2)^{1/2} \equiv i\hat{k}_\beta', & \omega/c < k_\parallel' \,, \quad (4.20\text{c}) \end{cases}$$

where $\hat{k}_1'$, $\hat{k}_\alpha'$, and $\hat{k}_\beta'$ are real.

In the interval $k_\parallel' > \omega/c$ we have to proceed carefully because of the pole in the integrand at the surface polariton dispersion relation. In fact, we have that

$$\frac{1}{k_1' - \epsilon(\omega)k'} = \frac{1}{\hat{k}_1' + \epsilon(\omega)\hat{k}_\beta'} = \frac{i[\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta']}{1-\epsilon^2(\omega)}\left(k_\parallel'^2 - \frac{\omega^2}{c^2}\frac{\epsilon(\omega)}{\epsilon(\omega)+1}\right)^{-1} . \tag{4.21}$$

If we now define the surface polariton wave vector $k_{sp}(\omega)$ by

$$k_{sp}^2(\omega) = \frac{\omega^2}{c^2}\frac{\epsilon(\omega)}{\epsilon(\omega)+1} \,, \tag{4.22}$$

we have the result that

$$\frac{1}{k_1' - \epsilon(\omega)k'} = i\frac{\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta'}{[1-\epsilon^2(\omega)][k_\parallel' + k_{sp}(\omega)]}\frac{1}{k_\parallel' - k_{sp}(\omega)} . \tag{4.23}$$

In order to define the manner in which we go around the pole in the integrand defined by Eq. (4.23) we recall that in fact $\epsilon(\omega)$ is complex [see Eqs. (4.1) and (4.2)], $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$, where $\epsilon_2(\omega) > 0$. Thus, we find that

$$k_{sp}(\omega) = k_{sp}^{(r)}(\omega) + ik_{sp}^{(i)}(\omega) \,, \tag{4.24}$$

where

$$k_{sp}^{(r)}(\omega) \cong \frac{\omega}{c}\left(\frac{\epsilon_1(\omega)[\epsilon_1(\omega)+1] + \epsilon_2^2(\omega)}{[\epsilon_1(\omega)+1]^2 + \epsilon_2^2(\omega)}\right)^{1/2} , \tag{4.25a}$$

$$k_{sp}^{(i)}(\omega) \cong \frac{\omega}{2c}\frac{\epsilon_2(\omega)}{\{[\epsilon_1(\omega)+1]^2 + \epsilon_2^2(\omega)\}^{1/2}\{\epsilon_1(\omega)[\epsilon_1(\omega)+1] + \epsilon_2^2(\omega)\}^{1/2}} \tag{4.25b}$$

and we have assumed $|\epsilon_2(\omega)| \ll 1$. In the frequency range where surface polaritons can exist, $k_{sp}^{(i)}$ is positive and very small in magnitude. Therefore, we will make the approximation that

$$\frac{1}{k_\parallel' - k_{sp}(\omega)} = \frac{1}{k_\parallel' - k_{sp}^{(r)}(\omega) - ik_{sp}^{(i)}(\omega)} \cong \frac{1}{[k_\parallel' - k_{sp}^{(r)}(\omega)]_P} + i\pi\delta(k_\parallel' - k_{sp}^{(r)}(\omega)), \tag{4.26}$$

where $1/(x)_P$ denotes the principal part of $1/x$. Finally we have that

$$\frac{1}{k_1' - \epsilon(\omega)k'}\,\frac{i[k_1' - \epsilon(\omega)k_\beta']}{1-\epsilon^2(\omega)} \times\left(\frac{1}{[k_\parallel'^2 - k_{sp}^{(r)}(\omega)^2]_P} + \frac{i\pi\delta(\hat{k}_\parallel' - k_{sp}^{(r)}(\omega))}{2k_{sp}^{(r)}(\omega)}\right) . \tag{4.27}$$

Having served the purpose of defining the manner in which the singularity in the integrand at $k_\parallel' = k_{sp}(\omega)$ is to be treated, the recognition that $\epsilon(\omega)$ is complex can in fact be forgotten in all that follows. We will treat $\epsilon(\omega)$ as real, being given by Eqs. (4.1) and (4.2) with $\gamma = 0$, and will take $k_{sp}(\omega)$ as given by Eq. (4.22) with this real $\epsilon(\omega)$.

With the preceding results in hand we can now write down the imaginary parts of $a(k_\parallel\omega), \ldots, e(k_\parallel\omega)$ for ω in the polariton regime $(\omega < ck_\parallel)$:

$$a^{(1)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' k_\parallel'\hat{k}_\alpha' \frac{k_\parallel'^2[2+\epsilon(\omega)] - 2\epsilon(\omega)(\omega^2/c^2)}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega) - k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \pi\left(\frac{\omega}{c}\right)^3 \frac{\epsilon^2(\omega)}{[\epsilon^2(\omega)-1][|\epsilon(\omega)|-1]^{3/2}} e^{-a^2k_{sp}^2(\omega)/4} I_0(\tfrac{1}{2}a^2k_\parallel k_{sp}(\omega))\right] , \tag{4.28a}$$

$$a^{(2)}(k_\parallel\omega) = -e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' k_\parallel' \frac{\hat{k}_1'\{k_\parallel'^2[1+2\epsilon(\omega)]-2\epsilon(\omega)(\omega^2/c^2)\}}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \int_{\omega/c}^{\infty} dk_\parallel' k_\parallel' \left(\frac{\hat{k}_1'\hat{k}_\beta'[\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta']}{[\epsilon^2(\omega)-1][k_\parallel'^2 - k_{sp}^2(\omega)]_P} + \frac{\omega^2}{c^2}\frac{1}{\hat{k}_1'+\hat{k}_\beta'}\right) e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel')\right], \quad (4.28b)$$

$$b^{(1)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' \frac{|\epsilon(\omega)|k_\parallel'^3\hat{k}_\alpha'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_2(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \pi\left(\frac{\omega}{c}\right)^3 \frac{\epsilon^2(\omega)}{[\epsilon^2(\omega)-1][|\epsilon(\omega)|-1]^{3/2}} e^{-a^2k_{sp}^2(\omega)/4} I_2(\tfrac{1}{2}a^2k_\parallel k_{sp}(\omega))\right], \quad (4.28c)$$

$$b^{(2)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' \frac{k_\parallel'^3\hat{k}_1'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_2(\tfrac{1}{2}a^2k_\parallel k_\parallel') - \int_{\omega/c}^{\infty} dk_\parallel' k_\parallel' \left(\frac{\hat{k}_\beta'\hat{k}_1'[\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta']}{[\epsilon^2(\omega)-1]^2[k_\parallel'^2 - k_{sp}^2(\omega)]_P} - \frac{\omega^2}{c^2}\frac{1}{\hat{k}_1'+\hat{k}_\beta'}\right) e^{-a^2k_\parallel'^2/4} I_2(\tfrac{1}{2}a^2k_\parallel k_\parallel')\right], \quad (4.28d)$$

$$c^{(1)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left(\int_0^{\omega/c} dk_\parallel' k_\parallel'^2\hat{k}_\alpha'^2 \frac{|\epsilon(\omega)|}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \int_{\omega/c}^{\infty} dk_\parallel' k_\parallel'^2 k_\beta' \frac{\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta'}{[\epsilon^2(\omega)-1][k_\parallel'^2 - k_{sp}^2(\omega)]_P} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}a^2k_\parallel k_\parallel')\right), \quad (4.28e)$$

$$c^{(2)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' \frac{k_\parallel'^2\hat{k}_\alpha'\hat{k}_1'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \pi\left(\frac{\omega}{c}\right)^3 \frac{|\epsilon(\omega)|^{3/2}}{[\epsilon^2(\omega)-1][|\epsilon(\omega)|-1]^{3/2}} e^{-a^2k_{sp}^2(\omega)/4} I_1(\tfrac{1}{2}a^2k_\parallel k_{sp}(\omega))\right], \quad (4.28f)$$

$$d^{(1)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left(\int_0^{\omega/c} dk_\parallel' \frac{k_\parallel'^2\hat{k}_1'^2}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}a^2k_\parallel k_\parallel') - \int_{\omega/c}^{\infty} dk_\parallel' \frac{k_\parallel'^2\hat{k}_1'[\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta']}{[\epsilon^2(\omega)-1][k_\parallel'^2 - k_{sp}^2(\omega)]_P} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}a^2k_\parallel k_\parallel')\right), \quad (4.28g)$$

$$d^{(2)}(k_\parallel\omega) = -e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' \frac{|\epsilon(\omega)|k_\parallel'^2\hat{k}_1'\hat{k}_\alpha'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_1(\tfrac{1}{2}k_\parallel k_\parallel') + \pi\left(\frac{\omega}{c}\right)^3 \frac{|\epsilon(\omega)|^{5/2}}{[\epsilon^2(\omega)-1][|\epsilon(\omega)|-1]^{3/2}} e^{-a^2k_{sp}^2(\omega)/4} I_1(\tfrac{1}{2}a^2k_\parallel k_{sp}(\omega))\right], \quad (4.28h)$$

$$e^{(1)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left[\int_0^{\omega/c} dk_\parallel' \frac{|\epsilon(\omega)|k_\parallel'^3\hat{k}_\alpha'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel') + \pi\left(\frac{\omega}{c}\right)^3 \frac{\epsilon^2(\omega)}{[\epsilon^2(\omega)-1][|\epsilon(\omega)|-1]^{3/2}} e^{-a^2k_{sp}^2(\omega)/4} I_0(\tfrac{1}{2}a^2k_\parallel k_{sp}(\omega))\right], \quad (4.28i)$$

$$e^{(2)}(k_\parallel\omega) = e^{-a^2k_\parallel^2/4}\left(\int_0^{\omega/c} dk_\parallel' \frac{k_\parallel'^3\hat{k}_1'}{[\epsilon^2(\omega)-1][k_{sp}^2(\omega)-k_\parallel'^2]} e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel') - \int_{\omega/c}^{\infty} dk_\parallel' \frac{k_\parallel'^3[\hat{k}_1' - \epsilon(\omega)\hat{k}_\beta']}{[\epsilon^2(\omega)-1][k_\parallel'^2 - k_{sp}^2(\omega)]_P} e^{-a^2k_\parallel'^2/4} I_0(\tfrac{1}{2}a^2k_\parallel k_\parallel')\right). \quad (4.28j)$$

In each case the first term is the contribution from the interval $0 \le k_\parallel' < \omega/c$, while the second is the contribution from the interval $k_\parallel' > \omega/c$.

In practice, a value of $k_\parallel$ was selected in units of ω_T/c for the dielectric constant (4.1) and in units of 10^{-4} Å^{-1} for the dielectric constant (4.2), and the corresponding value of $\omega_0(k_\parallel)$ was obtained from Eqs. (4.4) and (4.5), respectively. These values were then used in Eqs. (4.28), and the integration over $k_\parallel'$ was carried out by means of a 16 point Gaussian quadrature method. Good convergence of the integrals was obtained with this

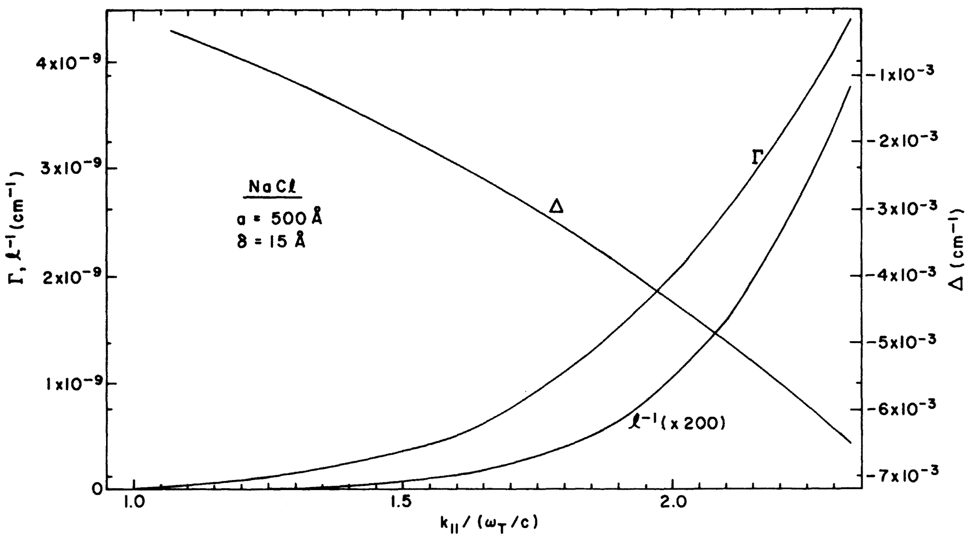

FIG. 3. Functions $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, $l^{-1}(k_\parallel)$ as functions of $k_\parallel$ for surface polaritons on a rough NaCl surface. Note that the graphical value of $l^{-1}(k_\parallel)$ is to be multiplied by 200.

number of points. Integrations carried out by this method using larger numbers of points gave the same results. The principal value integrals occurring in the integration over the range $\omega/c < k_\parallel' < \infty$ were evaluated by splitting the integration at the singularity,

$$P\int_{\omega/c}^{\infty} dk_\parallel' = \int_{\omega/c}^{k_{sp}-\epsilon} dk_\parallel' + \int_{k_{sp}+\epsilon}^{\infty} dk_\parallel' , \qquad (4.29)$$

and using a small, nonzero value for ϵ. The process was then repeated for a succession of values of $k_\parallel$. The resulting values of $a^{(1,2)}(k_\parallel\, \omega_0(k_\parallel)), \ldots, e^{(1,2)}(k_\parallel\, \omega_0(k_\parallel))$ were then combined according to Eqs. (4.19) to yield $G^{(1)}(k_\parallel \omega_0)$ and $G^{(2)}(k_\parallel \omega_0)$, when the values of $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, and $l^{-1}(k_\parallel)$ followed from Eqs. (4.15)–(4.17).

The results of these calculations are shown in Figs. 3–6. In Fig. 3 we present plots of $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, and $l^{-1}(k_\parallel)$ as functions of the dimensionless wave vector $k_\parallel/(\omega_T/c)$ for NaCl. The values of the parameters entering the dielectric constant (4.1) in this case are $\epsilon_0 = 5.9$, $\epsilon_\infty = 2.25$, $\omega_T = 164$ cm^{-1}, and $\omega_L = 264$ cm^{-1}. The transverse correlation length has been assumed to have the value $a = 500$ Å, and the root-mean-square deviation of the surface from flatness has been taken to be $\delta = 15$ Å. The range of values of $k_\parallel$ for which the results are plotted is approximately that which can be sampled by the attenuated-total-reflection method. For $k_\parallel/(\omega_T/c) = 2$, we see that $l^{-1} \cong 2.25\times 10^{-7}$ cm^{-1}, or $l = 4.4\times 10^{6}$ cm. The frequency shift $\Delta(k_\parallel)$ is seen to be negative and has a value of -4.4×10^{-3} cm^{-1}. The surface for which these calculations have been carried out is rather smooth, and the effects of surface roughness on surface polaritons are comparatively weak.

In Fig. 4 we have plotted the inverse attenuation length $l^{-1}(k_\parallel)$ against $k_\parallel(\omega_T/c)$ for a range of the latter which includes both the limit that $k_\parallel a \ll 1$ and that $k_\parallel a > 1$. It is seen that $l^{-1}(k_\parallel)$ passes through a maximum at a value of $k_\parallel$ for which $k_\parallel a \approx 1.5$, which is not unexpected on physical grounds and on the basis of the expressions for $a^{(1,2)}(k_\parallel \omega), \ldots, e^{(1,2)}(k_\parallel \omega)$ given by Eqs. (4.28). The minimum attenuation length in this case is $l(k_\parallel) \cong 6$ cm. This qualitative feature of the $k_\parallel$ dependence of $l^{-1}(k_\parallel)$ is in agreement with the results obtained by Mills.[7]

In Fig. 5 we present results for a much rougher surface of NaCl for the same range of wave vectors as in Fig. 3. In this case the surface is characterized by the parameters $a = \delta = 2500$ Å. It is seen that the magnitude of each of the functions $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, and $l^{-1}(k_\parallel)$ for this surface is considerably larger than in the case depicted in Fig. 3. Thus, for example, for $k_\parallel/(\omega_T/c) = 2$ we have that $l^{-1}(k_\parallel) \cong 0.15$ cm^{-1}, or $l(k_\parallel) \cong 6.6$ cm, while $\Delta(k_\parallel) \cong -23.5$ cm^{-1}. This is due largely to the proportionality of each of these quantities to $(\delta a)^2$, which factor has increased by 7×10^5 in going from Fig. 3 to Fig. 5. In Fig. 4 we have also plotted $l^{-1}(k_\parallel)$ over a wide range of $k_\parallel$, for $a = \delta = 2500$ Å, and we see that in this case as well this function has a maximum for $k_\parallel a \cong 1.5$. The minimum attenuation length in this case is $l(k_\parallel) \cong 5\times 10^{-5}$ cm.

In Fig. 6 we present results for the effects of surface roughness on surface polaritons on Al. The parameters entering the dielectric constant given by Eq. (4.2) were chosen to be $\epsilon_\infty = 1$ and $\omega_p = 1.2018\times 10^5$ cm^{-1}. The surface for which the calculations depicted in this figure were carried

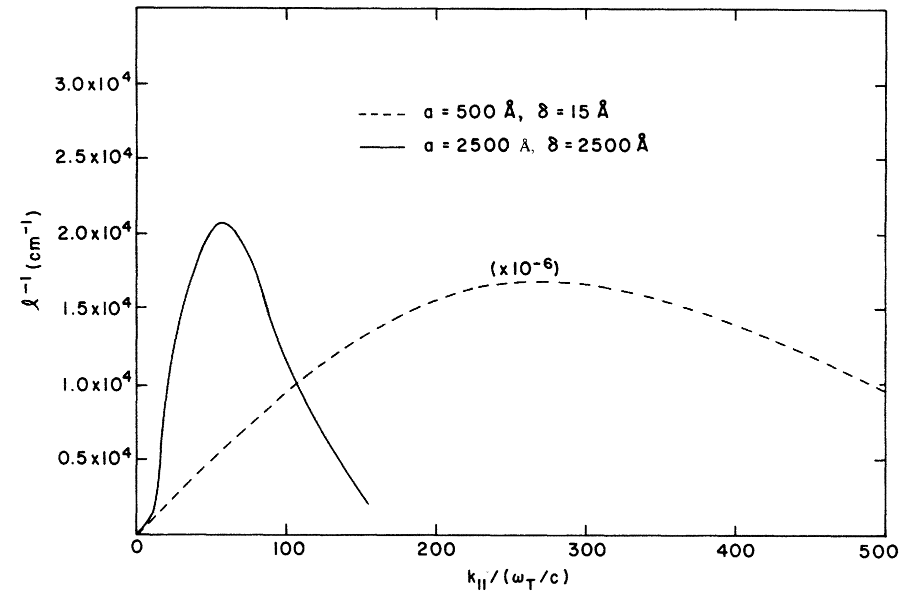

FIG. 4. Inverse attenuation length $l^{-1}(k_\parallel)$ for surface polaritons on two different rough NaCl surfaces. Note that the graphical value of $l^{-1}(k_\parallel)$ for the case $a=500$ Å, $\delta=15$ Å is to be multiplied by 10^{-6}.

out is rough, and is characterized by the values $a=\delta=2500$ Å. From this figure we find that for a wavelength of 2.1 μm ($k_\parallel = 3\times 10^{-4}$ Å^{-1}) $l^{-1}(k_\parallel) \cong 4\times 10^2$ cm^{-1}, so that $l(k_\parallel)\cong 2.5\times 10^{-3}$ cm. This result is in quantitative agreement with the predictions of the theory due to Mills.[7]

It is of interest to compare the contributions to the integrals defining the functions $a^{(1,2)}(k_\parallel\omega), \ldots, e^{(1,2)}(k_\parallel\omega)$ from the ranges $0\le k_\parallel' \le \omega/c$ and $\omega/c \le k_\parallel'$, which correspond, for example, to the attenuation of surface polaritons by roughness induced radiation into the vacuum and into other surface polaritons, respectively. Our numerical calculations show that the dominant contribution in each case arises from the range $\omega/c\le k_\parallel'$, i.e., the range corresponding to surface roughness induced scattering of a surface polariton into other surface polaritons. For $k_\parallel a \ll 1$ the contribution from the range $0\le k_\parallel' \le \omega/c$ is several orders of magnitude smaller than the contribution from the range $\omega/c\le k_\parallel'$, while for $k_\parallel' a \cong 1$ the two contributions are of the same order of magnitude. In the

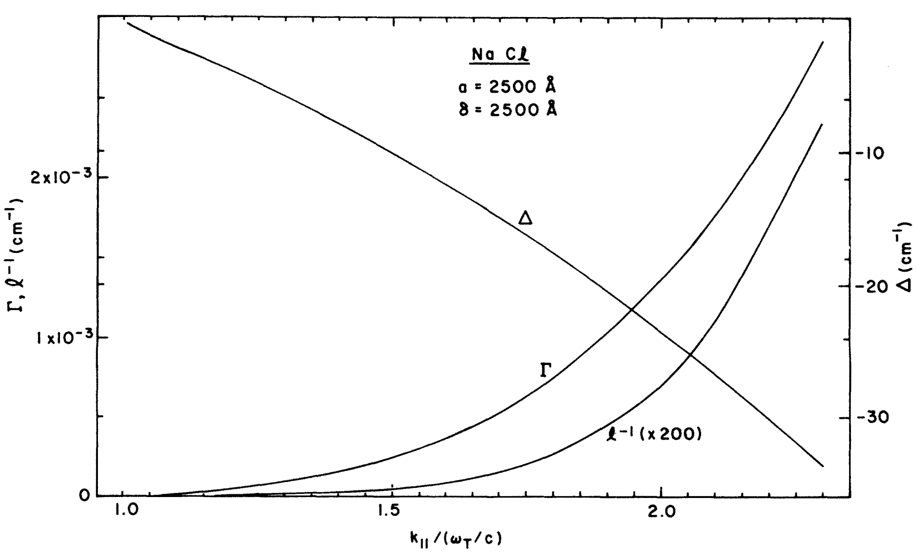

FIG. 5. Functions $\Delta(k_\parallel)$, $\Gamma(k_\parallel)$, $l^{-1}(k_\parallel)$ as functions of $k_\parallel$ for surface polaritons on a rough NaCl surface. Note that the graphical value of $l^{-1}(k_\parallel)$ is to be multiplied by 200.

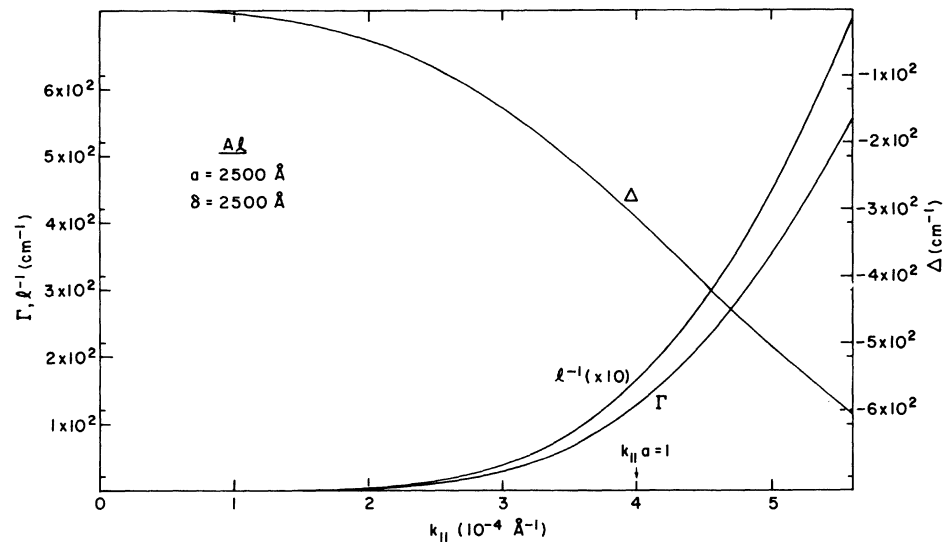

FIG. 6. Functions $\Delta(k_{\parallel})$, $\Gamma(k_{\parallel})$, $l^{-1}(k_{\parallel})$ as functions of $k_{\parallel}$ for surface polaritons on a rough Al surface. Note that the graphical value of $l^{-1}(k_{\parallel})$ is to be multiplied by 10.

case of Al, the difference between the contributions from the two ranges $0 \le k_{\parallel}' \le \omega/c$ and $\omega/c \le k_{\parallel}'$ is much smaller than in the case of NaCl. These results are in qualitative agreement with those obtained by Mills,[7] who finds that the surface scattering process dominates the radiation damping process in attenuating surface polaritons for values of $k_{\parallel}$, or of ω, for which $|\epsilon(\omega)| \lesssim 7$.

We also point out that the preceding results have been obtained on the assumption, sometimes explicit, mostly implicit that the frequency ω has an infinitesimal, positive imaginary part, $\omega \to \omega + i\eta$ ($\eta > 0$). If it is assumed that ω has an infinitesimal negative imaginary part, $\omega \to \omega - i\eta$, we find that

$$\epsilon(\omega - i\eta) = \epsilon^*(\omega + i\eta), \quad k(\omega - i\eta) = -k^*(\omega + i\eta), \quad k_1(\omega - i\eta) = -k_1^*(\omega + i\eta), \quad a(k_{\parallel}\omega - i\eta) = -a^*(k_{\parallel}\omega + i\eta),$$
$$b(k_{\parallel}\omega - i\eta) = -b^*(k_{\parallel}\omega + i\eta), \quad c(k_{\parallel}\omega - i\eta) = c^*(k_{\parallel}\omega + i\eta), \quad d(k_{\parallel}\omega - i\eta) = d^*(k_{\parallel}\omega + i\eta), \quad e(k_{\parallel}\omega - i\eta) = -e^*(k_{\parallel}\omega + i\eta). \tag{4.30}$$

Consequently, since

$$G(k_{\parallel}\omega + i\eta) = G^{(1)}(k_{\parallel}\omega) + iG^{(2)}(k_{\parallel}\omega) \,, \tag{4.31}$$

it follows that

$$G(k_{\parallel}\omega - i\eta) = -G^{(1)}(k_{\parallel}\omega) + iG^{(2)}(k_{\parallel}\omega) = -G^*(k_{\parallel}\omega + i\eta) \,. \tag{4.32}$$

These results are particularly useful in obtaining the Fourier transforms with respect to time of electric field correlation functions according to the methods of Refs. 8, 10, and 11.

Thus, we have presented a theory of the effects of surface roughness on the damping and frequency of a surface polariton, and in the process have obtained an explicit result for the Green's function for the Maxwell tensor differential operator in the presence of a rough surface, in terms of which electric field correlation functions arising in the theory of inelastic light scattering from excitations at a rough surface can be evaluated. From the results of numerical calculations based on the theory presented here, and the assumption that the Fourier coefficients of the surface roughness profile function are Gaussianly distributed random variables, it is possible to infer the degree of surface roughness that can be tolerated if a particular surface polariton mean free path is required at a given frequency. In all cases studied it is also found that surface roughness depresses the frequency of a surface polariton below its value in the absence of surface roughness. Experimental studies[5,6] of the attenuation and frequencies of surface polaritons in the presence of surface roughness would be valuable in checking the assumptions underlying the theory presented here.

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