Surface plasmons on a randomly rough surface

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We have studied the dispersion relation for surface plasmons on a randomly rough surface, going beyond the lowest-order approximation in the surface profile function. This improvement is required because an analysis of the expansion for the surface-plasmon dispersion relation in powers of the surface profile function shows that it contains an infinite subset of terms that are all of the same order of magnitude as the lowest-order contribution, which is the only one that has been considered in previous theoretical determinations of this dispersion relation. The indicated subset of terms is summed to yield a nonlinear integral equation for the surface-plasmon proper self-energy, in terms of which the dispersion relation is expressed. This integral equation has been solved numerically and the surface-plasmon spectral density constructed. The splitting of the surface-plasmon dispersion curve into two branches by the surface roughness, which was predicted theoretically by the lowest-order perturbation theory calculation, and which has been observed experimentally, is preserved in the results of the present calculation. However, both the magnitude of the splitting and the damping of the surface plasmon obtained from the present calculations are larger, for the same corrugation strength, than the same quantities obtained from the lowest-order perturbation calculation, for most surface-plasmon wave vectors.

I. INTRODUCTION

Recent theoretical[1–3] and experimental[4,5] studies have shown that the dispersion curve for surface plasmons propagating across a randomly rough dielectric surface consists of two branches, in contrast with the dispersion curve for surface plasmons on a flat surface which consists of a single, dispersionless branch.

This result was obtained theoretically in calculations in which the effects of the surface roughness were taken into account in only the lowest approximation in the surface profile function. In this paper we study the dispersion relation for surface plasmons on a randomly rough surface, going beyond this lowest-order approximation. This work was prompted by the fact that an examination of the higher-order terms in the expansion of the surface-plasmon dispersion relation in powers of the surface profile function revealed an infinite subset of terms that are all of the same order of magnitude as the lowest-order contribution, the only one considered in the previous theoretical determinations of this dispersion relation.[1–3]

As in our earlier studies of this problem[2,3] we work from the outset in the electrostatic approximation, and use the Rayleigh method[6] in solving Laplace's equation for the electrostatic potential in the dielectric medium and in the vacuum above it and satisfying the boundary conditions at the rough interface between them. However, in contrast with these earlier studies we use the extinction-theorem form of Green's theorem to eliminate the electrostatic potential in the dielectric medium. This leads to a single integral equation, for the Fourier transform of the potential in the vacuum, instead of the pair of coupled integral equations for the Fourier transforms of the potentials in both regions. The fact that we need to work with only a single integral equation greatly simplifies working to all orders in the surface profile function. The remainder of the analysis presented here is concerned with the transformation of this integral equation into an algebraic equation for the average of the Fourier transform of the electrostatic potential in the vacuum region over the ensemble of realizations of the surface profile, with the solvability condition for this equation, which yields the surface-plasmon dispersion relation, and with the solution of the dispersion relation.

We will find that the more refined treatment of the dispersion relation for surface plasmons on a randomly rough surface presented here leaves largely unchanged the qualitative results obtained in Refs. 1–3, but it does change them quantitatively.

The outline of this paper is as follows. We begin by characterizing a randomly rough surface in Sec. II. In Sec. III we obtain the integral equation for the Fourier transform of the electrostatic potential in the vacuum region above the dielectric medium that is valid to all orders in the surface-roughness profile function. This equation is solved to lowest nonzero order in the surface-roughness profile function in Sec. IV, and yields the surface-plasmon dispersion relation already obtained in Refs. 1–3. More importantly, this solution defines for us the subset of terms in the expansion of the dispersion relation to all orders in the surface profile function that are all of the same order as the one obtained in this small-roughness calculation. This subset of higher-order terms is summed in Sec. V to yield a nonlinear integral equation for the surface-plasmon proper self-energy, which is the principal ingredient in the surface-plasmon dispersion relation. In Sec. VI this integral equation is solved numerically, and the proper self-energy so obtained is used in a calculation of the surface-plasmon spectral density, whose peaks occur at the frequencies of surface plasmons on a randomly rough surface. A brief discussion of the results obtained, and of extensions of the work reported here, in Sec. VII, concludes this paper.

II. CHARACTERIZATION OF A RANDOMLY ROUGH SURFACE

The physical system we consider is depicted in Fig. 1. It consists of vacuum in the region $x_3 > \zeta(\vec{x}_{\parallel})$, and a dielectric medium characterized by an isotropic, frequency-dependent dielectric constant $\epsilon(\omega)$ in the region $x_3 < \zeta(\vec{x}_{\parallel})$. Here we have used the notation that $\vec{x}_{\parallel} = \hat{x}_1 x_1 + \hat{x}_2 x_2$, where $\hat{x}_1$ and $\hat{x}_2$ are unit vectors along the x_1 and x_2 directions.

The surface profile function $\zeta(\vec{x}_{\parallel})$ is a stationary stochastic process described by the statistical properties

$$\langle \zeta(\vec{x}_{\parallel}) \rangle = 0 , \tag{2.1a}$$

$$\langle \zeta(\vec{x}_{\parallel}) \zeta(\vec{x}_{\parallel}') \rangle = \delta^2 W(| \vec{x}_{\parallel} - \vec{x}_{\parallel}' |) , \tag{2.1b}$$

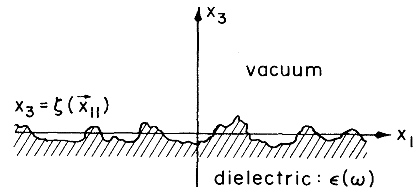

FIG. 1. Vacuum/dielectric system considered in this paper.

where the angular brackets denote an average over the ensemble of realizations of the surface profile, and δ^2 is the mean-square departure of the surface from flatness, $\delta^2 = \langle \zeta^2(\vec{x}_{\parallel}) \rangle$. We will make the additional assumption that $\zeta(\vec{x}_{\parallel})$ is a Gaussianly distributed random variable. This means that the average of the product of an odd number of factors of $\zeta(\vec{x}_{\parallel})$ with the same or different arguments vanishes, while the average of the product of an even number of factors of $\zeta(\vec{x}_{\parallel})$ is given by the sum of the products of the averages of $\zeta(\vec{x}_{\parallel})$'s paired two-by-two in all possible ways, e.g.,

$$\langle \zeta(\vec{x}_{\parallel}) \zeta(\vec{x}_{\parallel}') \zeta(\vec{x}_{\parallel}'') \zeta(\vec{x}_{\parallel}''') \rangle = \langle \zeta(\vec{x}_{\parallel}) \zeta(\vec{x}_{\parallel}') \rangle \langle \zeta(\vec{x}_{\parallel}'') \zeta(\vec{x}_{\parallel}''') \rangle + \langle \zeta(\vec{x}_{\parallel}) \zeta(\vec{x}_{\parallel}'') \rangle \langle \zeta(\vec{x}_{\parallel}') \zeta(\vec{x}_{\parallel}''') \rangle + \langle \zeta(\vec{x}_{\parallel}) \zeta(\vec{x}_{\parallel}''') \rangle \langle \zeta(\vec{x}_{\parallel}') \zeta(\vec{x}_{\parallel}'') \rangle . \tag{2.2}$$

The average of each pair of $\zeta(\vec{x}_{\parallel})$'s on the right-hand side of this equation, called a *contraction,* is given by Eq. (2.1b).

In what follows it will also be necessary to introduce the Fourier transform of the surface profile function $\zeta(\vec{x}_{\parallel})$,

$$\hat{\zeta}(\vec{k}_{\parallel}) = \int d^2x_{\parallel} e^{-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}} \zeta(\vec{x}_{\parallel}) . \tag{2.3}$$

We find from Eqs. (2.1) and (2.3) that

$$\langle \hat{\zeta}(\vec{k}_{\parallel}) \rangle = 0 , \tag{2.4a}$$

$$\langle \hat{\zeta}(\vec{k}_{\parallel}) \hat{\zeta}(\vec{k}_{\parallel}') \rangle = \delta^2 g(k_{\parallel}) (2\pi)^2 \delta(\vec{k}_{\parallel} + \vec{k}_{\parallel}') , \tag{2.4b}$$

where

$$g(k_{\parallel}) = \int d^2x_{\parallel} e^{-i\vec{k}_{\parallel}\cdot\vec{x}_{\parallel}} W(| \vec{x}_{\parallel} |) . \tag{2.5}$$

It follows from the assumption that $\zeta(\vec{x}_{\parallel})$ is a Gaussianly distributed random variable that the average of the product of an odd number of $\{\hat{\zeta}(\vec{k}_{\parallel})\}$ with the same or different arguments vanishes, while the average of the product of an even number of $\{\hat{\zeta}(\vec{k}_{\parallel})\}$ with the same or different arguments is given by the sum of products of the averages of $\hat{\zeta}(\vec{k}_{\parallel})$'s paired two-by-two in all possible ways, e.g.,

$$\langle \hat{\zeta}(\vec{k}_{\parallel}) \hat{\zeta}(\vec{k}_{\parallel}') \hat{\zeta}(\vec{k}_{\parallel}'') \hat{\zeta}(\vec{k}_{\parallel}''') \rangle = \langle \hat{\zeta}(\vec{k}_{\parallel}) \hat{\zeta}(\vec{k}_{\parallel}') \rangle \langle \hat{\zeta}(\vec{k}_{\parallel}'') \hat{\zeta}(\vec{k}_{\parallel}''') \rangle + \langle \hat{\zeta}(\vec{k}_{\parallel}) \hat{\zeta}(\vec{k}_{\parallel}'') \rangle \langle \hat{\zeta}(\vec{k}_{\parallel}') \hat{\zeta}(\vec{k}_{\parallel}''') \rangle + \langle \hat{\zeta}(\vec{k}_{\parallel}''') \hat{\zeta}(\vec{k}_{\parallel}) \rangle \langle \hat{\zeta}(\vec{k}_{\parallel}') \hat{\zeta}(\vec{k}_{\parallel}'') \rangle , \tag{2.6}$$

where each contraction is given by Eq. (2.4b).

III. THE EXTERNAL POTENTIAL

We seek the solution of Laplace's equation for the potential in each of the regions $x_3 \gtrless \zeta(\vec{x}_{\parallel})$,

$$\nabla^2 \phi^{>}(\vec{x} | \omega) = 0, \quad x_3 > \zeta(\vec{x}_{\parallel}) \tag{3.1a}$$

$$\nabla^2 \phi^{<}(\vec{x} | \omega) = 0, \quad x_3 < \zeta(\vec{x}_{\parallel}) \tag{3.1b}$$

subject to the boundary conditions,

$$\phi^{>}(\vec{x} | \omega) \big|_{x_3 = \zeta(\vec{x}_{\parallel})} = \phi^{<}(\vec{x} | \omega) \big|_{x_3 = \zeta(\vec{x}_{\parallel})} , \tag{3.2a}$$

$$\frac{\partial}{\partial n} \phi^{>}(\vec{x} | \omega) \bigg|_{x_3 = \zeta(\vec{x}_{\parallel})} = \epsilon(\omega) \frac{\partial}{\partial n} \phi^{<}(\vec{x} | \omega) \bigg|_{x_3 = \zeta(\vec{x}_{\parallel})} , \tag{3.2b}$$

at the interface $x_3=\zeta(\vec{x}_{\|})$, and the conditions

$$\phi^{\gtrless}(\vec{x}\,|\,\omega)\,|_{x_3=\pm\infty}=0 \tag{3.3}$$

at infinity, where the upper (lower) signs go together. In Eq. (2.4b) $\partial/\partial n$ is the derivative taken along the normal to the interface $x_3=\zeta(\vec{x}_{\|})$ at each point,

$$\frac{\partial}{\partial n}=\left[1+\left[\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_1}\right]^2+\left[\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_2}\right]^2\right]^{-1/2}\times\left[-\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_1}\frac{\partial}{\partial x_1}-\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_2}\frac{\partial}{\partial x_2}+\frac{\partial}{\partial x_3}\right], \tag{3.4}$$

when the normal is directed from the dielectric into vacuum.

The solution of Eq. (3.1a) in the region $x_3>\zeta(x_{\|})_{\max}$ that satisfies the boundary condition at infinity can be written in the form

$$\phi^{>}(\vec{x}\,|\,\omega)=\int\frac{d^2k_{\|}}{(2\pi)^2}A(\vec{k}_{\|},\omega)e^{i\vec{k}_{\|}\cdot\vec{x}_{\|}-k_{\|}x_3},\quad x_3>\zeta(\vec{x}_{\|})_{\max} \tag{3.5}$$

where $\vec{k}_{\|}=\hat{x}_1k_1+\hat{x}_2k_2$. A similar expression can be written for the potential in the region $x_3<\zeta(\vec{x}_{\|})_{\min}$, and the results used in the boundary conditions (3.2), according to the Rayleigh hypothesis.[6]

We will proceed differently here by eliminating the potential in the region $x_3<\zeta(\vec{x}_{\|})$ altogether, and working with the potential $\phi^{>}(\vec{x}\,|\,\omega)$ alone.

For this purpose we apply Green's theorem,

$$\int_V d^3x(u\nabla^2v-v\nabla^2u)=\int_\Sigma dS\left[u\frac{\partial v}{\partial n}-v\frac{\partial u}{\partial n}\right], \tag{3.6}$$

to the volume V defined by the region $x_3<\zeta(\vec{x}_{\|})$ occupied by the dielectric. The surface Σ bounding this volume consists of the interface $x_3=\zeta(\vec{x}_{\|})$ that we denote by S, and a hemispherical cap of infinite radius in the lower halfspace that we denote by $S^{(-\infty)}$. Since we are concerned with potentials $\phi^{<}(\vec{x}\,|\,\omega)$ that vanish exponentially as $x_3\to-\infty$ [Eq. (3.3)] the contribution to the right-hand side of Eq. (3.6) from the integral over $S^{(-\infty)}$ vanishes. The derivative $\partial/\partial n$ on the right-hand side of Eq. (3.6) is along the normal to the surface Σ directed outward from the volume V.

At this point we introduce the Green's function $G(\vec{x};\vec{x}')$ that is the solution of the equation

$$\nabla^2G(\vec{x};\vec{x}')=-4\pi\delta(\vec{x}-\vec{x}'), \tag{3.7}$$

subject to vanishing boundary conditions at infinity. A convenient representation for this function is

$$G(\vec{x};\vec{x}')=\int\frac{d^2q_{\|}}{(2\pi)^2}\frac{2\pi}{q_{\|}}e^{i\vec{q}_{\|}\cdot(\vec{x}_{\|}-\vec{x}'_{\|})}e^{-q_{\|}|x_3-x_3'|}. \tag{3.8}$$

We multiply Eq. (3.7) from the left by $\phi^{<}(\vec{x}\,|\,\omega)$ and subtract from the result the equation obtained by multiplying Eq. (3.1b) from the left by $G(\vec{x};\vec{x}')$. This difference is then integrated over the volume V, and use is made of Eq. (3.6). The result can be written as

$$\theta_V(\vec{x})\phi^{<}(\vec{x}\,|\,\omega)=-\frac{1}{4\pi}\int_S dS'\left[\left[\frac{\partial}{\partial n'}G(\vec{x};\vec{x}')\right]\phi^{<}(\vec{x}'\,|\,\omega)-G(\vec{x};\vec{x}')\frac{\partial}{\partial n'}\phi^{<}(\vec{x}'\,|\,\omega)\right], \tag{3.9}$$

where

$$\theta_V(\vec{x})=\int_V d^3x'\delta(\vec{x}-\vec{x}') \tag{3.10}$$

is unity if $\vec{x}\in V$ and vanishes if $\vec{x}\notin V$. In writing Eq. (3.9) we have used the symmetry of the Green's function, $G(\vec{x};\vec{x}')=G(\vec{x}';\vec{x})$. The normal derivative on the right-hand side of Eq. (3.9) is given by Eq. (3.4).

We now use the boundary conditions (3.2) and the assumption that $x_3>\zeta(\vec{x}_{\|})_{\max}$ to rewrite Eq. (3.9) as

$$0=-\frac{1}{4\pi}\int_S dS'\left[\left[\frac{\partial}{\partial n'}G(\vec{x};\vec{x}')\right]\phi^{>}(\vec{x}'\,|\,\omega)-\frac{1}{\epsilon(\omega)}G(\vec{x};\vec{x}')\frac{\partial}{\partial n'}\phi^{>}(\vec{x}'\,|\,\omega)\right],\quad x_3>\zeta(\vec{x}_{\|})_{\max}. \tag{3.11}$$

This is the boundary condition on $\phi^{>}(\vec{x}\,|\,\omega)$ that we will now use to determine the coefficient function $A(\vec{k}_{\|},\omega)$ in Eq. (3.5).

For this purpose it is convenient to go from integration over dS' in Eq. (3.11) to integration over $d^2x'_{\|}$ with the aid of the relation

$$dS=d^2x_{\|}\left[1+\left[\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_1}\right]^2+\left[\frac{\partial\zeta(\vec{x}_{\|})}{\partial x_2}\right]^2\right]^{1/2}. \tag{3.12}$$

The boundary condition (3.11) thus becomes

$$0=-\frac{1}{4\pi}\int d^2x'_{\|}\left[[\vec{n}'\cdot\vec{\nabla}'G(\vec{x};\vec{x}')]\phi^{>}(\vec{x}'\,|\,\omega)-\frac{1}{\epsilon(\omega)}G(\vec{x};\vec{x}')[\vec{n}'\cdot\vec{\nabla}'\phi^{>}(\vec{x}'\,|\,\omega)]\right]_{x_3'=\zeta(\vec{x}'_{\|})},\quad x_3>\zeta(\vec{x}_{\|})_{\max} \tag{3.13}$$

where

$$\vec{n}=\left[-\frac{\partial\zeta(\vec{x}_{||})}{\partial x_1},-\frac{\partial\zeta(\vec{x}_{||})}{\partial x_2},1\right] . \tag{3.14}$$

When we substitute Eqs. (3.5) and (3.8) into Eq. (3.13) we obtain

$$-\frac{1}{4\pi}\int d^2x'_{||}\int\frac{d^2q_{||}}{(2\pi)^2}\frac{2\pi}{q_{||}}e^{i\vec{q}_{||}\cdot\vec{x}_{||}-q_{||}x_3}e^{-i\vec{q}_{||}\cdot\vec{x}'_{||}+q_{||}\zeta(\vec{x}'_{||})}$$
$$\times\int\frac{d^2p_{||}}{(2\pi)^2}A(\vec{p}_{||},\omega)e^{i\vec{p}_{||}\cdot\vec{x}'_{||}-p_{||}\zeta(\vec{x}'_{||})}\left\{\vec{n}'\cdot\left[-i\left[\vec{q}_{||}+\frac{1}{\epsilon(\omega)}\vec{p}_{||}\right]\right.\right.$$
$$\left.\left.+\hat{x}_3\left[q_{||}+\frac{1}{\epsilon(\omega)}p_{||}\right]\right]\right\}=0,\quad x_3>\zeta(\vec{x}_{||})_{\max} . \tag{3.15}$$

To proceed farther we introduce the representation

$$e^{\alpha\zeta(\vec{x}_{||})}=\int\frac{d^2Q_{||}}{(2\pi)^2}I(\alpha\,|\,\vec{Q}_{||})e^{i\vec{Q}_{||}\cdot\vec{x}_{||}} , \tag{3.16}$$

where

$$\begin{aligned}I(\alpha\,|\,\vec{Q}_{||})&=\int d^2x_{||}e^{-i\vec{Q}_{||}\cdot\vec{x}_{||}}e^{\alpha\zeta(\vec{x}_{||})}\\&=(2\pi)^2\delta(\vec{Q}_{||})+\int d^2x_{||}e^{-i\vec{Q}_{||}\cdot\vec{x}_{||}}(e^{\alpha\zeta(\vec{x}_{||})}-1)\\&\equiv(2\pi)^2\delta(\vec{Q}_{||})+\alpha J(\alpha\,|\,\vec{Q}_{||}) .\end{aligned} \tag{3.17}$$

It follows from Eqs. (3.16) and (3.17) that

$$\frac{\partial\zeta(\vec{x}_{||})}{\partial x_\beta}e^{\alpha\zeta(\vec{x}_{||})}=\int\frac{d^2Q_{||}}{(2\pi)^2}iQ_\beta J(\alpha\,|\,\vec{Q}_{||})e^{i\vec{Q}_{||}\cdot\vec{x}_{||}},\quad \beta=1,2 . \tag{3.18}$$

When the results given by Eqs. (3.16)—(3.18) are used in Eq. (3.15) we obtain

$$\int\frac{d^2q_{||}}{(2\pi)^2}e^{i\vec{q}_{||}\cdot\vec{x}_{||}}\frac{e^{-q_{||}x_3}}{2q_{||}}A(\vec{q}_{||},\omega)q_{||}\left[1+\frac{1}{\epsilon(\omega)}\right]$$
$$+\int\frac{d^2q_{||}}{(2\pi)^2}e^{i\vec{q}_{||}\cdot\vec{x}_{||}}\frac{e^{-q_{||}x_3}}{2q_{||}}\int\frac{d^2p_{||}}{(2\pi)^2}A(\vec{p}_{||},\omega)J(q_{||}-p_{||}\,|\,\vec{q}_{||}-\vec{p}_{||})$$
$$\times[(-i\vec{q}_{||}+q_{||}\hat{x}_3)+(i\vec{p}_{||}-p_{||}\hat{x}_3)]\cdot\left[(-i\vec{q}_{||}+q_{||}\hat{x}_3)-\frac{1}{\epsilon(\omega)}(i\vec{p}_{||}-p_{||}\hat{x}_3)\right]=0 ,$$
$$x_3>\zeta(\vec{x}_{||})_{\max} . \tag{3.19}$$

On equating to zero the $\vec{q}_{||}$-th Fourier coefficient in this equation we obtain finally the integral equation satisfied by $A(\vec{q}_{||},\omega)$:

$$\frac{\epsilon(\omega)+1}{\epsilon(\omega)-1}A(\vec{q}_{||},\omega)+\int\frac{d^2p_{||}}{(2\pi)^2}J(q_{||}-p_{||}\,|\,\vec{q}_{||}-\vec{p}_{||})(\hat{q}_{||}\cdot\hat{p}_{||}-1)p_{||}A(\vec{p}_{||},\omega)=0 . \tag{3.20}$$

IV. SMALL-ROUGHNESS LIMIT

Before proceeding to a detailed investigation of Eq. (3.20) we first examine it in the small-roughness limit to show that it yields the result of earlier studies of the present problem,[1-3] and to motivate the work that follows.

The small-roughness limit is obtained by retaining only the lowest nonvanishing term in the expansion of $J(\alpha\,|\,\vec{Q}_{||})$ in powers of $\zeta(\vec{x}_{||})$:

$$\begin{aligned}J(\alpha\,|\,\vec{Q}_{||})&=\frac{1}{\alpha}\int d^2x_{||}e^{-i\vec{Q}_{||}\cdot\vec{x}_{||}}(e^{\alpha\zeta(\vec{x}_{||})}-1)\\&=\int d^2x_{||}e^{-i\vec{Q}_{||}\cdot\vec{x}_{||}}[\zeta(\vec{x}_{||})+\tfrac{1}{2}\alpha\zeta^2(\vec{x}_{||})+\tfrac{1}{6}\alpha^2\zeta^3(\vec{x}_{||})+\cdots]\\&=\hat{\zeta}^{(1)}(\vec{Q}_{||})+\tfrac{1}{2}\alpha\hat{\zeta}^{(2)}(\vec{Q}_{||})+\tfrac{1}{6}\alpha^2\hat{\zeta}^{(3)}(\vec{Q}_{||})+\cdots ,\end{aligned} \tag{4.1}$$

where

$$\hat{\zeta}^{(n)}(\vec{Q}_{||})=\int d^2x_{||}e^{-i\vec{Q}_{||}\cdot\vec{x}_{||}}\zeta^n(\vec{x}_{||}) . \quad (4.2)$$

The coefficients $\{\hat{\zeta}^{(n)}(\vec{Q}_{||})\}$ can be calculated recursively according to

$$\hat{\zeta}^{(1)}(\vec{Q}_{||})\equiv\hat{\zeta}(\vec{Q}_{||}) , \quad (4.3a)$$

$$\hat{\zeta}^{(n+1)}(\vec{Q}_{||})=\int\frac{d^2P_{||}}{(2\pi)^2}\hat{\zeta}^{(n)}(\vec{Q}_{||}-\vec{P}_{||})\hat{\zeta}(\vec{P}_{||}) . \quad (4.3b)$$

Thus, in the small-roughness limit Eq. (3.20) becomes

$$A(\vec{q}_{||}\omega)=\frac{1}{\gamma(\omega)}\int\frac{d^2p_{||}}{(2\pi)^2}\hat{\zeta}(\vec{q}_{||}-\vec{p}_{||}) \times(1-\vec{q}_{||}\cdot\vec{p}_{||})p_{||}A(\vec{p}_{||},\omega) , \quad (4.4)$$

where we have introduced the notation

$$\gamma(\omega)=\frac{\epsilon(\omega)+1}{\epsilon(\omega)-1} . \quad (4.5)$$

Because $\zeta(\vec{x}_{||})$ is a random function so is the solution $A(\vec{q}_{||},\omega)$ of Eq. (4.4). Just as $\zeta(\vec{x}_{||})$ is defined by its moments, viz. by Eqs. (2.1) and the assumption that it is a Gaussianly distributed random variable, so $A(\vec{q}_{||},\omega)$ can be defined by its moments. Of these a particularly important one is $\langle A(\vec{q}_{||},\omega)\rangle$ which, through Eq. (3.5), determines the average potential in the region $x_3>\zeta(\vec{x}_{||})_{\max}$ depicted in Fig. 1. It is to the determination of this function that we now turn.

To this end we introduce the smoothing operator P that averages everything it acts on over the ensemble of realizations of the surface profile,

$$Pf=\langle f\rangle . \quad (4.6)$$

The complementary operator $Q=1-P$ projects out the fluctuating part of anything it acts on. We apply the operator P to both sides of Eq. (4.4) to obtain

$$PA(\vec{q}_{||},\omega)=\frac{1}{\gamma(\omega)}\int\frac{d^2p_{||}}{(2\pi)^2}p_{||}(1-\hat{q}_{||}\cdot\hat{p}_{||}) \times P\hat{\zeta}(\vec{q}_{||}-\vec{p}_{||})QA(\vec{p}_{||},\omega) . \quad (4.7)$$

In writing this equation we have used the identity $A=(P+Q)A$, and the result that $P\hat{\zeta}(\vec{q}_{||}-\vec{p}_{||})=0$ [see Eq. (2.4a)]. We next apply the operator Q to both sides of Eq. (4.4) and find

$$QA(\vec{p}_{||},\omega)=\frac{1}{\gamma(\omega)}\int\frac{d^2Q_{||}}{(2\pi)^2}Q_{||}(1-\hat{p}_{||}\cdot\hat{Q}_{||}) \times\hat{\zeta}(\vec{p}_{||}-\vec{Q}_{||})PA(\vec{Q}_{||},\omega) , \quad (4.8)$$

where we have neglected a term $Q\hat{\zeta}(\vec{p}_{||}-\vec{Q}_{||})QA(\vec{Q}_{||},\omega)$ as of second order in $\zeta(\vec{x}_{||})$, and have again used the fact that $P\hat{\zeta}(\vec{p}_{||}-\vec{Q}_{||})=0$. We now substitute Eq. (4.8) into Eq. (4.7) with the result that

$$\gamma^2(\omega)\langle A(\vec{q}_{||},\omega)\rangle =\int\frac{d^2p_{||}}{(2\pi)^2}\int\frac{d^2Q_{||}}{(2\pi)^2}p_{||}Q_{||}(1-\hat{q}_{||}\cdot\hat{p}_{||})(1-\hat{p}_{||}\cdot\hat{Q}_{||}) \times\langle\hat{\zeta}(\vec{q}_{||}-\vec{p}_{||})\hat{\zeta}(\vec{p}_{||}-\vec{Q}_{||})\rangle\langle A(\vec{Q}_{||},\omega)\rangle . \quad (4.9)$$

With the use of Eq. (2.4b) in Eq. (4.9) we immediately obtain the dispersion relation for surface plasmons on a randomly rough surface in the form

$$\gamma^2(\omega)=\delta^2\int\frac{d^2p_{||}}{(2\pi)^2}q_{||}p_{||}(1-\hat{q}_{||}\cdot\hat{p}_{||})^2g(|\vec{q}_{||}-\vec{p}_{||}|) . \quad (4.10)$$

This is just the dispersion relation that is obtained by combining Eqs. (4.127) and (4.129) of Ref. 3, and retaining only terms of $0(\delta^2)$. If we rewrite Eq. (4.10) as

$$\gamma(\omega)=\pm\delta\left[\int\frac{d^2p_{||}}{(2\pi)^2}q_{||}p_{||}(1-\hat{q}_{||}\cdot\hat{p}_{||})^2 \times g(|\vec{q}_{||}-\vec{p}_{||}|)\right]^{1/2} , \quad (4.11)$$

then we see that to every solution of the equation

$$\gamma(\omega)=0 , \quad (4.12)$$

which is the dispersion relation for surface plasmons on a planar surface, correspond two solutions of the dispersion relation for surface plasmons on a randomly rough surface. This is the roughness-induced splitting of the surface-plasmon dispersion curve mentioned in the Introduction.

In all that follows we will assume that the correlation function $W(|\vec{x}_{||}|)$ has the Gaussian form[7]

$$W(|\vec{x}_{||}|)=e^{-x_{||}^2/a^2} , \quad (4.13)$$

where the quantity a is called the *transverse correlation length,* so that $g(k_{||})$ is given by

$$g(k_{||})=\pi a^2e^{-k_{||}^2a^2/4} . \quad (4.14)$$

Equation (4.11) then takes the form

$$\gamma(\omega)=\pm(\delta/a)\sqrt{2}f(\xi) , \quad (4.15)$$

where

$$f(\xi)=\frac{1}{\xi}\left[e^{-\xi^2/4}\int_0^\infty du\,u^2e^{-u^2/\xi^2}[3I_0(u)-2I_1(u) +I_2(u)]\right]^{1/2} , \quad (4.16)$$

with $\xi=q_{||}a$ and $I_n(x)$ a modified Bessel function of the first kind. The function $f(\xi)$ has been evaluated, and Eq. (4.15) solved, in Ref. 2. More important from the standpoint of the present work is the result obtained there that

$\sqrt{2}f(\xi)$ is of order unity over a broad range of ξ (from $\xi \sim 0.1$ to $\xi \sim 4$). This means, from Eq. (4.15), that at resonance $\gamma(\omega)$ is of $O(\delta/a)$, or equivalently $(\delta/a)/\gamma(\omega)$ is of $O(1)$. It should be emphasized that this result is independent of our assumption that $W(|\vec{x}_{||}|)$ has the Gaussian form (4.13). The choice of any other correlation function that decreases significantly from unity with increasing $|\vec{x}_{||}|$ over a characteristic distance a will yield a result of the form given by Eq. (4.15). Of course the coefficient of (δ/a) will have a different dependence on ξ from the one given by Eq. (4.16), but it will still be of order unity over a broad range of ξ. An example of this is presented in Ref. 2. We will see in the next section that if we retain terms of all order in the surface profile function in obtaining the surface-plasmon dispersion relation from Eq. (3.20), we will encounter an infinite subset of terms, of which the nth is proportional to $(\delta/a)^n/\gamma(\omega)^n$, and hence is of the same order of magnitude at resonance as the lowest-order term that gives rise to Eq. (4.4). It is therefore incorrect to retain only the lowest-order term in $(\delta/a)/\gamma(\omega)$ from this infinite subset of terms: Since all the rest are of the same order of magnitude they must all be taken into account in obtaining the dispersion relation. It is to this that the next section is devoted.

V. SURFACE-PLASMON DISPERSION RELATION TO LEADING ORDER IN $\delta/\gamma(\omega)$

We now return to Eq. (3.20) with the aim of obtaining from it the equation satisfied by $\langle A(\vec{q}_{||},\omega)\rangle$ that is not limited by the retention of only the first term in the expansion of $J(\alpha|\vec{Q}_{||})$ in powers of $\zeta(\vec{x}_{||})$, given by Eq. (4.1). For this it is convenient to rewrite Eq. (3.20) in the form

$$A(\vec{q}_{||},\omega)-\int \frac{d^2p_{||}}{(2\pi)^2}K(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)A(\vec{p}_{||},\omega)=0\ , \qquad (5.1)$$

where the kernel of this equation can be expanded in powers of $\zeta(\vec{x}_{||})$ according to

$$\begin{aligned}K(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)&=\gamma^{-1}(\omega)J(q_{||}-p_{||}\,|\,\vec{q}_{||}-\vec{p}_{||})(1-\hat{q}_{||}\cdot\hat{p}_{||})p_{||}\\ &=\sum_{n=1}^{\infty}\frac{(q_{||}-p_{||})^{n-1}}{n!}\frac{\hat{\zeta}^{(n)}(\vec{q}_{||}-\vec{p}_{||})}{\gamma(\omega)}(1-\vec{q}_{||}\cdot\vec{p}_{||})p_{||}\\ &=\sum_{n=1}^{\infty}K^{(n)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)\ .\end{aligned} \qquad (5.2)$$

In the nonzero averages to which it contributes $\hat{\zeta}^{(n)}(\vec{k}_{||})$ is of $O(\delta^n)$, according to Eqs. (4.2), (2.4b), and (2.7), and the assumption that $\zeta(\vec{x}_{||})$ is a Gaussianly distributed random variable. Consequently, $K^{(n)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ has the order of magnitude $\delta^n/\gamma(\omega)\sim\delta^{n-1}$.

If we now apply the operators P and Q to Eq. (5.1) in turn and extract from the results the equation satisfied by $PA(\vec{q}_{||},\omega)$ we find that it is

$$\langle A(\vec{q}_{||},\omega)\rangle-\int \frac{d^2p_{||}}{(2\pi)^2}\langle M(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)\rangle\langle(A(\vec{p}_{||},\omega)\rangle=0\ , \qquad (5.3)$$

where $M(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ is the solution of the integral equation,

$$M(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)=K(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)+\int \frac{d^2r_{||}}{(2\pi)^2}K(\vec{q}_{||};\vec{r}_{||}\,|\,\omega)QM(\vec{r}_{||};\vec{p}_{||}\,|\,\omega)\ . \qquad (5.4)$$

If we solve Eq. (5.4) by iteration and average the resulting series term-by-term, it is clear from the definition (5.2) and the order estimate that follows that all the terms in $\langle M(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)\rangle$ of $O((\delta/a)^n/\gamma^n(\omega))$ and hence of $O(1)$ are obtained if we replace $K(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ in Eq. (5.4) by $K^{(1)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$. The resulting approximation to $M(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ will be denoted by $M^{(0)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$, because it is of zero net order in δ. It satisfies the equation

$$M^{(0)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)=K^{(1)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)+\int \frac{d^2r_{||}}{(2\pi)^2}K^{(1)}(\vec{q}_{||};\vec{r}_{||}\,|\,\omega)QM^{(0)}(\vec{r}_{||};\vec{p}_{||}\,|\,\omega)\ , \qquad (5.5)$$

where

$$K^{(1)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)=\hat{\zeta}(\vec{q}_{||}-\vec{p}_{||})(1-\hat{q}_{||}\cdot\hat{p}_{||})\frac{p_{||}}{\gamma(\omega)}\ . \qquad (5.6)$$

We now proceed to solve Eq. (5.5) by iteration and average the resulting series term-by-term with the aid of Eqs. (2.4b) and the assumption that $\zeta(\vec{x}_{||})$ is a Gaussianly distributed random variable. Only terms containing $K^{(1)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ an even number of times survive averaging due to the latter assumption.

The second-order contribution to $\langle M^{(0)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)\rangle$ is given by

$$\int \frac{d^2p_{\parallel}^{(1)}}{(2\pi)^2} \langle K^{(1)}(\vec{q}_{\parallel};\vec{p}_{\parallel}^{(1)}\,|\,\omega) Q K^{(1)}(\vec{p}_{\parallel}^{(1)};\vec{p}_{\parallel}\,|\,\omega)\rangle$$

$$=(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{p}_{\parallel})\frac{q_{\parallel}}{\gamma(\omega)}\int \frac{d^2p_{\parallel}^{(1)}}{(2\pi)^2}(1-\hat{q}_{\parallel}\cdot\hat{p}_{\parallel}^{(1)})\delta^2 g(\,|\,\vec{q}_{\parallel}-\vec{p}_{\parallel}^{(1)}\,|\,)\frac{p_{\parallel}^{(1)}}{\gamma(\omega)}(1-\hat{p}_{\parallel}^{(1)}\cdot\hat{q}_{\parallel}) \,. \quad (5.7)$$

The fourth-order contribution consists of two terms:

$$\int \frac{d^2p_{\parallel}^{(1)}}{(2\pi)^2}\int \frac{d^2p_{\parallel}^{(2)}}{(2\pi)^2}\int \frac{d^2p_{\parallel}^{(3)}}{(2\pi)^2}\langle K^{(1)}(\vec{q}_{\parallel};\vec{p}_{\parallel}^{(1)}\,|\,\omega)QK^{(1)}(\vec{p}_{\parallel}^{(1)};\vec{p}_{\parallel}^{(2)}\,|\,\omega)QK^{(1)}(\vec{p}_{\parallel}^{(2)};\vec{p}_{\parallel}^{(3)}\,|\,\omega)QK^{(1)}(\vec{p}_{\parallel}^{(3)};\vec{p}_{\parallel}\,|\,\omega)\rangle$$

$$= (2\pi)^2\delta(\vec{q}_{\parallel}-\vec{p}_{\parallel})\frac{q_{\parallel}}{\gamma(\omega)}\int \frac{d^2p_{\parallel}^{(1)}}{(2\pi)^2}\int \frac{d^2p_{\parallel}^{(2)}}{(2\pi)^2}(1-\hat{q}_{\parallel}\cdot\hat{p}_{\parallel}^{(2)})$$

$$\times\left[1-\hat{p}_{\parallel}\cdot\frac{\vec{p}_{\parallel}^{(1)}+\vec{p}_{\parallel}^{(2)}-\vec{q}_{\parallel}}{|\,\vec{p}_{\parallel}^{(1)}+\vec{p}_{\parallel}^{(2)}-\vec{q}_{\parallel}\,|}\right]\left[1-\frac{\vec{p}_{\parallel}^{(1)}+\vec{p}_{\parallel}^{(2)}-\vec{q}_{\parallel}}{|\,\vec{p}_{\parallel}^{(1)}+\vec{p}_{\parallel}^{(2)}-\vec{q}_{\parallel}\,|}\cdot\hat{p}_{\parallel}^{(1)}\right](1-\hat{p}_{\parallel}^{(1)}\cdot\hat{q}_{\parallel})$$

$$\times\frac{p_{\parallel}^{(1)}}{\gamma(\omega)}\frac{p_{\parallel}^{(2)}}{\gamma(\omega)}\frac{|\,\vec{p}_{\parallel}^{(1)}+\vec{p}_{\parallel}^{(2)}-\vec{q}_{\parallel}\,|}{\gamma(\omega)}\delta^2 g(\,|\,\vec{q}_{\parallel}-\vec{p}_{\parallel}^{(2)}\,|\,)\delta^2 g(\,|\,\vec{q}_{\parallel}-\vec{p}_{\parallel}^{(1)})$$

$$+(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{p}_{\parallel})\frac{q_{\parallel}}{\gamma(\omega)}\int \frac{d^2p_{\parallel}^{(1)}}{(2\pi)^2}\int \frac{d^2p_{\parallel}^{(2)}}{(2\pi)^2}(1-\hat{q}_{\parallel}\cdot\hat{p}_{\parallel}^{(1)})(1-\hat{p}_{\parallel}^{(1)}\cdot\hat{p}_{\parallel}^{(2)})$$

$$\times(1-\hat{p}_{\parallel}^{(2)}\cdot\hat{p}_{\parallel}^{(1)})(1-\hat{p}_{\parallel}^{(1)}\cdot\hat{q}_{\parallel})\frac{p_{\parallel}^{(1)}}{\gamma(\omega)}\frac{p_{\parallel}^{(2)}}{\gamma(\omega)}\frac{p_{\parallel}^{(1)}}{\gamma(\omega)}$$

$$\times\delta^2 g(\,|\,\vec{q}_{\parallel}-\vec{p}_{\parallel}^{(1)}\,|\,)\delta^2 g(\,|\,\vec{p}_{\parallel}^{(2)}-\vec{p}_{\parallel}^{(1)}\,|\,) \,. \quad (5.8)$$

In these two results we see two features that are in fact general properties of $\langle M^{(0)}(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)\rangle$ (and more generally of $\langle M(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)\rangle$). The first is the presence of the factor $(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{p}_{\parallel})$ in each term. This arises from the fact that the averaging process restores infinitesimal translational invariance to our system. The second is the presence of the factor $q_{\parallel}/\gamma(\omega)$ in each term. This arises from the structure of the kernel $K(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)$, and of its lowest-order approximation $K^{(1)}(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)$, and from the aforementioned restoration of translational invariance. In what follows we will therefore write $\langle M(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)\rangle$ as

$$\langle M(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)\rangle=(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{p}_{\parallel})\frac{q_{\parallel}}{\gamma(\omega)}\Sigma(\vec{q}_{\parallel},\omega) \,. \quad (5.9)$$

When the result given by Eq. (5.9) is substituted into Eq. (5.3), the dispersion relation for surface plasmons on a randomly rough surface becomes

$$1=\frac{q_{\parallel}}{\gamma(\omega)}\Sigma(\vec{q}_{\parallel},\omega) \,. \quad (5.10)$$

Thus, in what follows we will focus our attention on the function $\Sigma(\vec{q}_{\parallel},\omega)$, in particular on the approximation to it, $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$, that is obtained when $K(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)$ is replaced by $K^{(1)}(\vec{q}_{\parallel};\vec{p}_{\parallel}\,|\,\omega)$. The terms in the series for $\Sigma(\vec{q}_{\parallel},\omega)$ can be represented by diagrams,[8] and it will prove convenient to do so.

Thus, the second-order contribution to $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$ obtained from Eq. (5.7) can be represented by Fig. 2, while the two fourth-order contributions are represented by Figs. 3(a) and 3(b). The rules for constructing these diagrams, and all diagrams of higher order in $\zeta(\vec{x}_{\parallel})$ contributing to $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$ are as follows. On a horizontal solid line mark off $2n$ dots (vertices) (for a diagram of $2n$th order). Label the portion of this horizontal line to the left of the leftmost vertex by the wave vector $\vec{q}_{\parallel}$, and label the portion to the right of the rightmost vertex also by $\vec{q}_{\parallel}$. Join the $2n$ vertices pairwise by dashed lines in all possible ways (subject to a restriction to be mentioned below). Label the portions of the horizontal solid line between consecutive vertices, and the dashed lines, by wave vectors

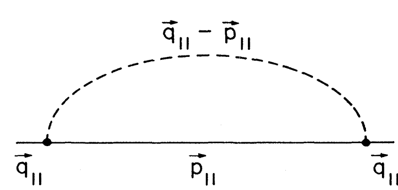

FIG. 2. Diagrammatic representation of the second-order contribution to $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$ arising from Eq. (5.7).

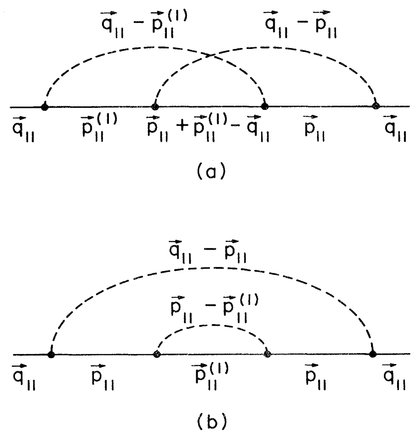

FIG. 3. Diagrammatic representation of the two fourth-order contributions to $\Sigma^0(\vec{q}_{\parallel}\omega)$ arising from Eq. (5.8).

subject to the rule that the sum of the wave vectors entering a vertex must equal the sum of the wave vectors leaving the vertex. (For this purpose it is convenient to assume that all solid and dashed lines are directed from left to right.) With a horizontal solid line labeled by a wave vector $\vec{p}_{\parallel}$ we associate a factor $p_{\parallel}/\gamma(\omega)$. However, no factors $q_{\parallel}/\gamma(\omega)$ are to be associated with the incoming and outgoing lines labeled by the wave vector $\vec{q}_{\parallel}$. With a dashed line labeled by a wave vector $\vec{q}_{\parallel}$ we associate a factor $\delta^2 g(|\vec{q}_{\parallel}|)$. With each vertex, bordered by horizontal straight line segments labeled by wave vectors $\vec{p}_{\parallel}$ and $\vec{p}\,'_{\parallel}$, we associate a factor $(1-\hat{p}_{\parallel}\cdot\hat{p}'_{\parallel})$. For convenience in what follows we adopt the convention of labeling the last horizontal solid line entering the rightmost dot from the left by $\vec{p}_{\parallel}$, and the dashed line entering this dot by $\vec{q}_{\parallel}-\vec{p}_{\parallel}$. Finally, the free wave vectors, $\vec{p}_{\parallel},\vec{p}_{\parallel}^{\,(1)},\ldots$, are to be integrated with volume elements $d^2p_{\parallel}/(2\pi)^2, d^2p_{\parallel}^{(1)}/(2\pi)^2,\ldots$, respectively.

There is one restriction that must be imposed on the preceding rules. It is already observed in Figs. 3(a) and 3(b). This is that in pairing vertices with dashed lines no pairing is allowed that gives rise to a diagram that can be separated into two pieces by cutting a single, horizontal line (that must necessarily be labeled by the wave vector $\vec{q}_{\parallel}$). Thus, only proper diagrams are to be considered, and $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$ therefore has the nature of a proper self-energy. This restriction comes about due to the presence of the operator Q in the kernel of Eq. (5.5) and consequently in expressions such as those given by Eqs. (5.7) and (5.8). An alternative way of understanding this result is through adding a source term $(2\pi)^2\delta(\vec{q}_{\parallel}-\vec{q}_{\parallel}^{\,(0)})q_{\parallel}/\gamma(\omega)$ to the right-hand side of Eq. (5.1). In this case $\langle A(\vec{q}_{\parallel},\omega)\rangle$ can be renamed $\langle G(\vec{q}_{\parallel};\vec{q}_{\parallel}^{\,0}|\omega)\rangle$ and is found to satisfy the Dyson equation

$$\langle G(\vec{q}_{\parallel};\overset{0}{\vec{q}}_{\parallel}|\omega)\rangle = G_0(\vec{q}_{\parallel};\overset{0}{\vec{q}}_{\parallel}|\omega) + \int \frac{d^2p_{\parallel}}{(2\pi)^2} G_0(\vec{q}_{\parallel};\vec{p}_{\parallel}|\omega)\Sigma(\vec{p}_{\parallel},\omega) \times \langle G(\vec{p}_{\parallel};\overset{0}{\vec{q}}_{\parallel}|\omega)\rangle , \tag{5.11}$$

in which $G_0(\vec{q}_{\parallel};\overset{0}{\vec{q}}_{\parallel}|\omega)=(2\pi)^2\delta(\vec{q}_{\parallel}-\overset{0}{\vec{q}}_{\parallel})q_{\parallel}/\gamma(\omega)$ plays the role of the unperturbed propagator and $\Sigma(\vec{q}_{\parallel},\omega)$ is the corresponding self-energy. The diagrams of sixth order in $\zeta(\vec{x}_{\parallel})$ contributing to $\Sigma^{(0)}(\vec{q}_{\parallel},\omega)$ are depicted in Fig. 4.

From the results depicted in Figs. 2–4 we see that the interactions depicted by the dashed lines contribute self-energy insertions to the "bare propagators" depicted by the horizontal solid line segments, labeled, e.g., by $p_{\parallel}/\gamma(\omega)$. A self-energy insertion is a portion of a diagram that can be excised from it by cutting two horizontal solid lines. We can simplify the subsequent analysis by considering only diagrams with no self-energy insertions (skeleton diagrams) provided that the horizontal solid lines in these diagrams are replaced by doubled solid lines. With such a doubled solid line labeled by a wave vector $\vec{q}_{\parallel}$ we associate a factor $G(\vec{q}_{\parallel},\omega)$ that is the solution of the Dyson equation

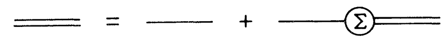

FIG. 5. The diagrammatic depiction of the Dyson equation (5.12).

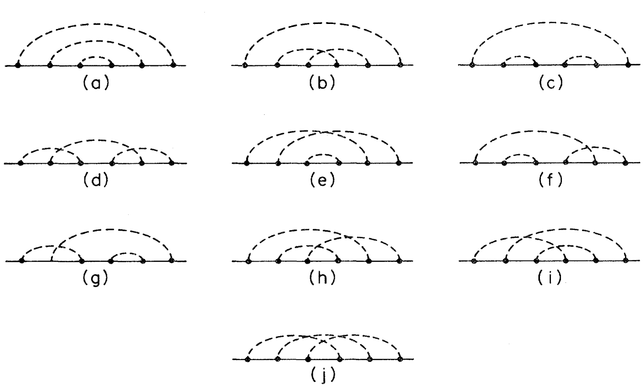

FIG. 4. Diagrammatic representation of the ten sixth-order contributions to $\Sigma^{(0)}(\vec{q}_{\parallel}\omega)$.

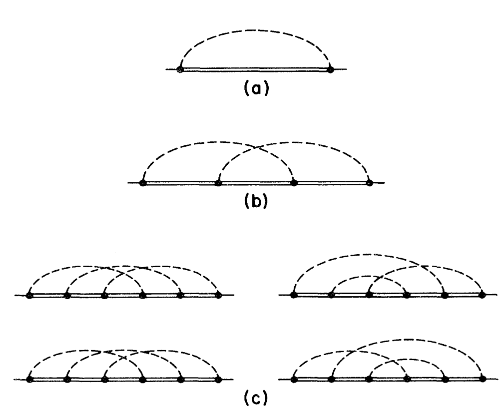

FIG. 6. Skeleton diagrams of (a) second-, (b) fourth-, and (c) sixth-order contributing to $\Sigma^{(0)}(\vec{q}_{\parallel}\omega)$.

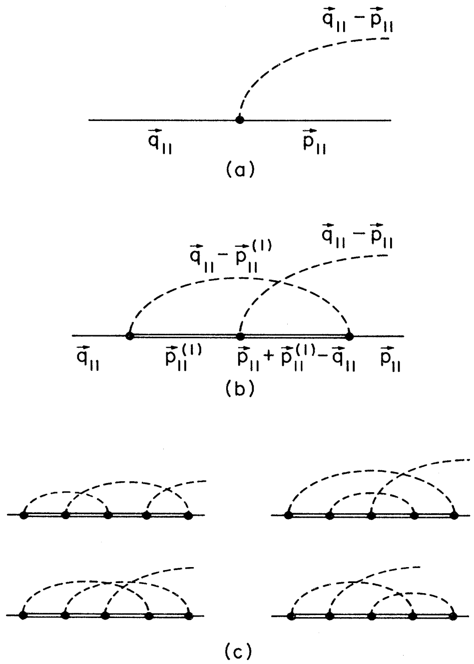

FIG. 7. Diagrammatic depiction of the (a) first-, (b) third-, and (c) fifth-order contributions to the vertex function $\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)$.

$$G(\vec{q}_{\|},\omega)=\frac{q_{\|}}{\gamma(\omega)}+\frac{q_{\|}}{\gamma(\omega)}\Sigma^{(0)}(\vec{q}_{\|},\omega)G(\vec{q}_{\|},\omega)\ , \quad (5.12)$$

that is depicted graphically in Fig. 5. The remaining rules for calculating a contribution to $\Sigma^{(0)}(\vec{q}_{\|},\omega)$ are unchanged.

The lowest-order skeleton diagrams contributing to $\Sigma^{(0)}(\vec{q}_{\|},\omega)$ are depicted in Fig. 6. From these diagrams we see that the interactions depicted by the dashed lines also renormalize the left-hand vertex. (One could equally well take the point of view that they renormalize the right-hand vertex or even that they renormalize both the right-hand and left-hand vertices. The subsequent analysis is simplified, however, if it is assumed that only one of the vertices is renormalized, and we choose it to be the left-hand vertex.) This vertex renormalization can be taken into account by introducing the vertex function $\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)$ whose lowest-order contributions are depicted diagrammatically in Fig. 7. The rules for obtaining a contribution to the vertex function $\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)$ are as follows. On a horizontal solid-line segment mark off $2n+1$ dots (vertices) for a vertex function of $(2n+1)$th order. Label the line entering the leftmost vertex by $\vec{q}_{\|}$, and the line leaving the rightmost vertex by $\vec{p}_{\|}$. Draw a dashed line labeled by $\vec{q}_{\|}-\vec{p}_{\|}$ leaving any vertex and pair the remaining $2n$ vertices by dashed lines in all possible ways, provided that the resulting diagrams are proper diagrams and contain no self-energy insertions. Wave vectors are conserved at each vertex as before, and a horizontal solid-line segment labeled by $\vec{p}_{\|}^{(i)}$ is represented by $G(\vec{p}_{\|}^{(i)}\omega)$ while a dashed line labeled by $\vec{p}_{\|}^{(i)}$ is represented by $\delta^2 g(\,|\vec{p}_{\|}^{(i)}|\,)$. Each vertex is depicted by $(1-\hat{p}_{\|}^{(i)}\cdot\hat{p}_{\|}^{(j)})$, where $\vec{p}_{\|}^{(i)}$ and $\vec{p}_{\|}^{(j)}$ label the solid lines entering and leaving it. The solid lines labeled by $\vec{q}_{\|}$ and $\vec{p}_{\|}$ and the dashed line labeled by $\vec{q}_{\|}-\vec{p}_{\|}$ make no contribution to $\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)$, however. All free wave vectors are then integrated over.

The first-order contribution to $\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)$ depicted in Fig. 7(a) is simply $(1-\hat{q}_{\|}\cdot\hat{p}_{\|})$. The third-order contribution depicted in Fig. 7(b) is given by

$$\int\frac{d^2p_{\|}^{(1)}}{(2\pi)^2}(1-\hat{q}_{\|}\cdot\hat{p}_{\|}^{(1)})\left[1-\hat{p}_{\|}^{(1)}\cdot\frac{(\vec{p}_{\|}+\vec{p}_{\|}^{(1)}-\vec{q}_{\|})}{|\vec{p}_{\|}+\vec{p}_{\|}^{(1)}-\vec{q}_{\|}|}\right]\left[1-\frac{(\vec{p}_{\|}+\vec{p}_{\|}^{(1)}-\vec{q}_{\|})}{|\vec{p}_{\|}+\vec{p}_{\|}^{(1)}-\vec{q}_{\|}|}\cdot\hat{p}_{\|}\right]$$
$$\times G(\vec{p}_{\|}^{(1)},\omega)G(\vec{p}_{\|}+\vec{p}_{\|}^{(1)}-\vec{q}_{\|},\omega)\delta^2 g(\,|\vec{q}_{\|}-\vec{p}_{\|}^{(1)}|\,)\ . \quad (5.13)$$

The infinite-order perturbation series for $\Sigma^{(0)}(\vec{q}_{\|},\omega)$ can now be summed formally to yield the highly nonlinear integral equation for $\Sigma^{(0)}(\vec{q}_{\|},\omega)$:

$$\Sigma^{(0)}(\vec{q}_{\|},\omega)=\int\frac{d^2p_{\|}}{(2\pi)^2}\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)\delta^2 g(\,|\vec{q}_{\|}-\vec{p}_{\|}|\,)G(\vec{p}_{\|},\omega)(1-\hat{p}_{\|}\cdot\hat{q}_{\|})$$
$$=\int\frac{d^2p_{\|}}{(2\pi^2)}\frac{\Gamma(\vec{q}_{\|};\vec{p}_{\|}\,|\,\omega)\delta^2 g(\,|\vec{q}_{\|}-\vec{p}_{\|}|\,)(1-\hat{p}_{\|}\cdot\hat{q}_{\|})}{\gamma(\omega)/p_{\|}-\Sigma^{(0)}(\vec{p}_{\|},\omega)}\ . \quad (5.14)$$

VI. NUMERICAL RESULTS

In this section we describe the numerical solution of the integral equation (5.14). The manner of solution was dictated by the manner in which we elected to present our results. We have chosen to construct the surface-plasmon spectral density

$$\rho(\vec{q}_{\|},\omega)=\frac{1}{2\pi i}[G(\vec{q}_{\|},\omega+i0)-G(\vec{q}_{\|},\omega-i0)]$$
$$=\frac{q_{\|}}{\pi}\frac{q_{\|}\Sigma_I^{(0)}(\vec{q}_{\|},\omega)+\gamma_I(\omega)}{[\gamma_R(\omega)-q_{\|}\Sigma_R^{(0)}(\vec{q}_{\|},\omega)]^2+[q_{\|}\Sigma_I^{(0)}(\vec{q}_{\|},\omega)+\gamma_I(\omega)]^2}\ , \quad (6.1)$$

where we have used Eq. (5.12) and the definitions

$$\gamma(\omega \pm i0) = \gamma_R(\omega) \mp i\gamma_I(\omega) , \tag{6.2a}$$

$$\Sigma^{(0)}(\vec{q}_{||},\omega \mp i0) = \Sigma_R^{(0)}(\vec{q}_{||},\omega) \pm i\Sigma_I^{(0)}(\vec{q}_{||},\omega) . \tag{6.2b}$$

Equation (6.2a) follows from the definition of $\gamma(\omega)$, Eq. (4.5), and the result that $\epsilon(\omega \pm i0) = \epsilon_R(\omega) \pm i\epsilon_I(\omega)$. The spectral density $\rho(\vec{q}_{||}\omega)$ for a given value of $\vec{q}_{||}$ has peaks at the values of ω for which the dispersion relation (5.10) has a solution when ω is replaced by $\omega + i0$.

To solve Eq. (5.14) for $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ we have to make some approximation for the vertex function $\Gamma(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$. We have chosen to approximate it by the lowest-order approximation, viz. $(1-\vec{q}_{||}\cdot\vec{p}_{||})$. This is because, in the absence of an exact evaluation of the third-order contribution to $\Gamma(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ given by Eq. (5.13), estimates of it in the limit that both $q_{||}$ and $p_{||}$ are small compared with a^{-1}, and in the limit that both are large compared with a^{-1}, in the approximation that $G(\vec{q}_{||},\omega)$ is replaced by $g_{||}/\gamma(\omega)$, show that it is small compared with $(1-\hat{q}_{||}\cdot\hat{p}_{||})$. The results we obtain in these limits are

$$\Gamma(\vec{q}_{||};\vec{p}_{||}\,|\,\omega) \sim \begin{cases} \dfrac{(\delta^2/a^2)}{4\gamma^2(\omega)}[(aq_{||}-ap_{||})^2(1+\tfrac{1}{4}\cos\theta)+\tfrac{1}{2}(aq_{||})(ap_{||})(1-\cos\theta)(5+2\cos\theta)], & aq_{||},ap_{||} \ll 1 \quad (6.3a) \\ \dfrac{(\delta^2/a^2)}{\gamma^2(\omega)}\dfrac{1}{(aq_{||})(ap_{||})}(1-\cos\theta)(1+2\cos^2\theta), & aq_{||},ap_{||} \gg 1 \quad (6.3b) \end{cases}$$

where we have set $\hat{q}_{||}\cdot\hat{p}_{||} = \cos\theta$. In fact, it is the former result that is the more significant one because of the factor $\exp(-\frac{1}{4}a^2q_{||}^2 - \frac{1}{4}a^2p_{||}^2)$ appearing in the integrand of Eq. (5.14) through the presence of the surface structure factor $g(|\vec{q}_{||}-\vec{p}_{||}|)$. Although the smallness of $\Gamma(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ [compared with $(1-\hat{q}_{||}\cdot\hat{p}_{||})$] in these two limits does not guarantee its relative smallness for all $q_{||}$ and $p_{||}$, it is suggestive of it, and in what follows we will assume that this is the case.

The integral equation for $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ in this approximation thus takes the form

$$\Sigma^{(0)}(\vec{q}_{||},\omega+i0) = \frac{a^2\delta^2}{4\pi}e^{-a^2q_{||}^2/4}\int_0^\infty dp_{||}p_{||}^2 e^{-1/4a^2p_{||}^2}\int_{-\pi}^{\pi} d\theta \frac{(1-\cos\theta)^2 e^{(a^2q_{||}p_{||}\cos\theta/2)}}{\gamma(\omega+i0)-p_{||}\Sigma^{(0)}(\vec{p}_{||},\omega+i0)} , \tag{6.4}$$

where we have used Eq. (4.14), and have measured the azimuthal angle θ from the direction of $\vec{q}_{||}$.

It is also necessary to make a choice for the form of the dielectric constant $\epsilon(\omega)$. In the present work we used the free-electron metal form, $\epsilon(\omega) = 1-(\omega_p^2/\omega^2)$, where ω_p is the plasmon frequency for the conduction electrons in the bulk of the metal. For this choice of $\epsilon(\omega)$ the function $\gamma(\omega)$ takes the form

$$\gamma(\omega) = 1-2\omega^2/\omega_p^2 . \tag{6.5}$$

The zero of this function, which is the frequency of a surface plasmon at a planar vacuum-metal interface, is given by the well-known expression

$$\omega_{sp} = \omega_p/\sqrt{2} . \tag{6.6}$$

Equation (6.4) was solved by iteration. To start the iteration $\Sigma^{(0)}(\vec{p}_{||},\omega+i0)$ was assumed to be identically zero in the integrand on the right-hand side of Eq. (6.4). The angular integration was carried out analytically and the integration over $p_{||}$ was carried out numerically, by Simpson's rule, to yield a first approximation to $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ that is clearly a function of $\vec{q}_{||}$ only through its magnitude. This result was then substituted into the right-hand side of Eq. (6.6) and the process repeated until a converged result for $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ was obtained. Since at every stage of the iterative solution $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ depends on $\vec{q}_{||}$ only through its magnitude, we carried out the angular integration analytically to obtain Eq. (6.4) in the more convenient form

$$S^{(0)}(\xi,\omega+i0) = \frac{\delta^2}{4a^2}e^{-\xi^2/4}\int_0^\infty dx \frac{x^2e^{-x^2/4}}{\gamma(\omega+i0)-xS^{(0)}(x,\omega+i0)}[3I_0(\tfrac{1}{2}\xi x)-4I_1(\tfrac{1}{2}\xi x)+I_2(\tfrac{1}{2}\xi x)] , \tag{6.7}$$

where we have set $\xi = aq_{||}$, and

$$\Sigma^{(0)}(q_{||},\omega+i0) = aS^{(0)}(\xi,\omega+i0) . \tag{6.8}$$

In the calculations based on Eq. (6.7) the positive infinitesimal imaginary part of ω that we have denoted by $+i0$ was represented by $+i\eta$, where η was taken to be $10^{-4}\omega_{sp}$.

The result that $\Sigma^{(0)}(\vec{q}_{||},\omega+i0)$ is a function of $\vec{q}_{||}$ only through its magnitude is a reflection of the fact that, with the form of the two-point correlation function given by

Eq. (2.1b), averaging the electrostatic scalar potential over the ensemble of realizations of the surface profile function restores isotropy in the plane $x_3=0$ to the system we are studying.

Two results for the dimensionless surface-plasmon spectral density $\hat{\rho}(\xi,\omega)=a\rho(q_{\|},\omega)$ are shown in Fig. 8, together with the result obtained in the lowest-order approximation, $S^{(0)}(\xi,\omega+i0)\equiv 0$, of Refs. 1–3. The value of ξ chosen in these calculations, viz. $\xi=1$, is the result for which the maximum splitting of the surface-plasmon dispersion curve in the latter approximation occurs. It is seen that the spectral density obtained on the basis of the self-consistent result for $S^{(0)}(\xi,\omega+i0)$ resembles the result obtained in the lowest-order approximation in displaying two peaks, signifying the roughness-induced splitting of the surface-plasmon dispersion curve into two branches. However, the magnitude of the splitting, as measured by the distance between the centers of the two peaks, is significantly increased in the results based on the self-consistent calculation of $S^{(0)}(\xi,\omega+i0)$ over the splitting obtained in the lowest-order approximation. To obtain a splitting of 0.15–0.2 eV in the surface-plasmon dispersion curve for Ag, as has been observed experimentally by Kotz *et al.*[5] a value of $\delta/a\cong 0.05$ is required for $\xi=1$ on the basis of the present results.

At the same time, each of the two peaks in the spectral density is significantly broadened in comparison with the peaks obtained in the lowest-order approximation. Indeed, in the latter approximation the peaks are rigorously δ functions. The widths they display in Figs. 8, and their finite amplitudes, are due to the replacement of $\omega+i0$ by $\omega+i\eta$ in the numerical calculations, where η is small but finite. The widths of the peaks in the spectral density in the present work are due to the attenuation of the surface plasmon as it propagates along a randomly rough surface by its roughness-induced multiple scattering into the surface plasmons, which removes energy from the incident beam. In addition, the spectral density acquires a significant nonzero value in the frequency range between the two peaks, where it is zero in the lowest-order approximation. This, too, is in qualitative agreement with the experimental results.[4]

Finally, in Fig. 9 we have plotted the frequencies of the two peaks in the spectral density as functions of ξ, together with the dispersion curves obtained in the lowest order

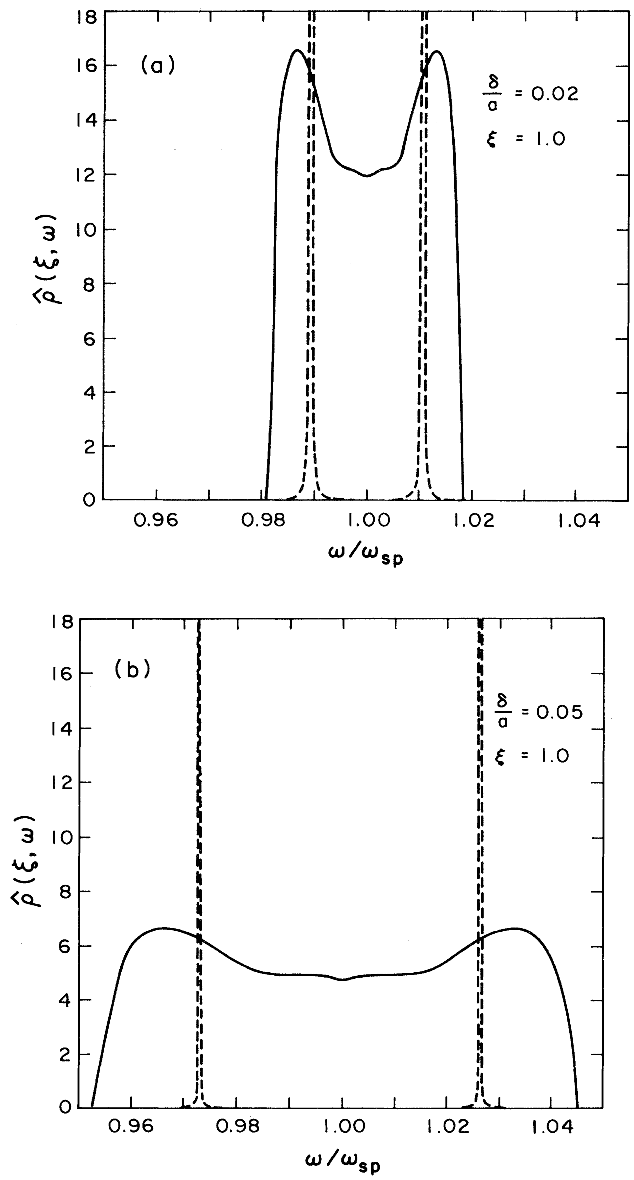

FIG. 8. Spectral density of surface plasmons on a randomly rough surface calculated self-consistently (solid line), and in the lowest-order approximation in the surface profile function (dashed line), at $\xi=1$, for two values of δ/a: (a) $\delta/a=0.02$; (b) $\delta/a=0.05$.

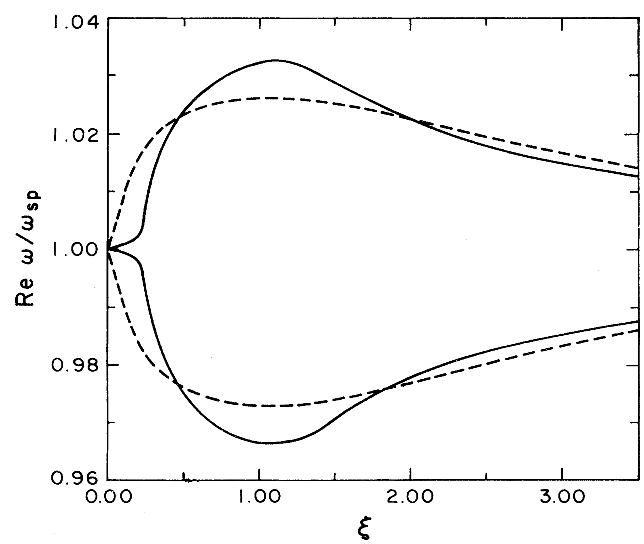

FIG. 9. Frequencies of surface plasmons on a randomly rough surface as obtained from the positions of the peaks in the spectral density Eq. (6.1) (solid line), and from the lowest order approximation in the surface profile function (dashed line), for $\delta/a=0.05$.

for $\delta/a = 0.05$. It is seen that the splitting of the dispersion curve obtained in the present calculations exceeds that calculated in the lowest-order approximation for $0.3 \lesssim \xi < 2$.

VII. DISCUSSION

Although the results of the present self-consistent calculation of the proper self-energy of a surface plasmon on a randomly rough surface and those of the lowest-order approximation may not differ significantly for frequencies far from resonance, where $\gamma(\omega)$ is no longer of $O(\delta/a)$, but instead is of $O(\delta^2/a^2)$, there are significant differences between them in the resonance region, i.e., for frequencies in the vicinity of the peaks in the spectral density. These differences are manifested in a slightly larger splitting between the two branches of the surface-plasmon dispersion curve, and a much larger damping of the surface plasmon, for a given value of the corrugation strength δ/a and dimensionless wave vector $\xi = q_{||}a$. The results of the present calculations show, for the first time, the necessity of including contributions of the form of $[(\delta/a)/\gamma(\omega)]^n$ for all n in calculations of resonant properties of surface plasmons on randomly rough surfaces.

Surface plasmons at a planar metal/vacuum interface are comparatively unusual among surface excitations in having a dispersion curve that is dispersionless, i.e., independent of both the magnitude and direction of the two-dimensional wave vector characterizing their propagation across the interface. It is this feature of their dispersion curve that is ultimately responsible for its splitting into two branches at a randomly rough metal/vacuum interface,[1,2] and consequently for the result that $\gamma(\omega)$ is of $O(\delta/a)$ at resonance, which underlies the present work. Surface excitations whose dispersion curves are wave-vector dependent do not display roughness-induced splittings. The summation of higher-order terms in the determination of the corresponding self-energies, of the kind carried out in this paper, is therefore not expected to have dramatic consequences for the frequencies of these excitations. The situation with respect to the lifetimes of such excitations may be quite different, however. The results of the present work, which show that a self-consistent calculation of the self-energy of a surface plasmon yields a significant increase of its imaginary part over the value obtained from the lowest-order-perturbation theoretic calculation, suggests that a similar result may be obtained for dispersive surface excitations as well.

It would therefore be of considerable interest to reexamine the determinations of the dispersion curve for surface polaritons on a randomly rough surface by Kretschmann and Kroger,[9] Maradudin and Zierau,[8] and Toigo *et al.*,[10] from this point of view. A first step in this direction has been taken by Haller,[11] but in this work approximations were made in deriving the nonlinear integral equation for the surface-polariton self-energy, and additional work on this problem remains to be done.

At the same time the propagation of Rayleigh-surface acoustic waves[12–15] and of shear horizontal surface acoustic waves[16,17] across randomly rough surfaces has been studied theoretically, as well as the energy levels of electrons in a thin film with one randomly rough surface,[18] and magnetic surface excitations on a randomly rough surface,[19,20] plasmons in a randomly rough sphere,[21] electronic energy levels in randomly rough spheres[21,22] and polaritons in randomly rough cylinders.[23] In each of these calculations only the contribution to the corresponding self-energy of lowest nonzero order in the surface profile $\zeta(\vec{x}_{||})$ was kept. It seems likely that a recalculation of these self-energies in the resonance region by the kind of infinite-order perturbation calculation presented here would lead to rather smaller mean-free paths for the corresponding surface excitations than are predicted by the existing calculations.

A worthwhile topic for further study in the context of such calculations is the extent to which vertex corrections can be incorporated into them. It seems clear that $\Gamma(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$ is a function of $\vec{q}_{||}$ and $\vec{p}_{||}$ only through the magnitudes of these wave vectors and of the cosine of the angle between them, and this result may serve as the basis for a systematic approximation scheme for the inclusion of vertex corrections.

Finally, we note that recent calculations of the dispersion curves of surface plasmons on deterministic, periodically corrugated surfaces[24,25] revealed an infinite number of branches in these curves, disposed essentially symmetrically about the (dispersionless) dispersion curve for plasmons on a flat surface. To obtain such a multiplicity of branches in the present calculation it is necessary to retain the higher-order terms, $K^{(2)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega)$, $K^{(3)}(\vec{q}_{||};\vec{p}_{||}\,|\,\omega), \ldots$ in the expansion (5.2) of the kernel in the integral equation (5.1). Such a calculation has not been carried out yet.

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