Improved method for calculating the dispersion of surface excitations in inhomogeneous media

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We propose a continued-fraction technique which relates logarithmic derivatives of a function defined by a second-order differential equation at a matching surface. We use this method as a general scheme for finding the dispersion relation for surface excitations. As a particular example we show that the dispersion relation for surface plasmons in an inhomogeneous conductor arises naturally without assumptions about the dielectric function chosen, or the validity of a power-series solution near a singularity.

I. INTRODUCTION

Given the atomic nature of matter, an interface between two phases must have nonzero thickness. It then follows that the properties of a phase close to an interface must be inhomogeneous to some extent, e.g., the conductivity of a liquid metal is likely dependent on distance from the surface in some transition zone at the surface. The study of surface plasma waves at a dielectric inhomogeneous conducting interface[1-3] has generated a novel prediction. An analysis of the local behavior of surface excitations leads to two branches in the spectrum, whereas when the conductor is homogeneous only one branch can exist.[4] The existence of the second branch in the surface-plasmon dispersion has been attributed to the interference between two kinds of excitations at the interface. Experimental verification for the existence of this second branch has been obtained from studies of attenuated total reflection from the liquid alloy Hg-Cs.[5]

The theoretical interpretation of the attenuated total reflection follows from an examination of the solutions of Maxwell's equations on either side of the inhomogeneity, and the conditions that each solution must satisfy at the interface. To be more specific, the discontinuity "seen" by the photon is due to the change in the dielectric properties of the composite dielectric-conducting alloy system. It has usually been assumed that the conductivity of the alloy changes from its value at the surface to its value in the bulk with an exponential dependence on distance from the surface, where surface refers to the plane of contact between the alloy and the dielectric. The permittivity of the nonconducting dielectric does not vary with distance from the surface, and it has a value which is different from that of the alloy at the surface. Elementary electrodynamical arguments predict reflection at this surface with changes in the field amplitudes governed by the boundary conditions. Discontinuities of waves across a surface produce dispersion relations which, for this problem, will relate the wave vector to the frequency of the field amplitude.

A second-order differential equation describing the magnetic field amplitudes provides a general description of the system described, including the relevant physics.[3] Following the introduction of a specific form for the dependence of the dielectric function on distance from the surface—an exponential in the case previously studied—this differential equation is analyzed by means of locally valid representations of the solutions on both sides of the discontinuity. From the matching relations for the electric and magnetic fields at the surface, the relevant dispersion relation is obtained; for the case cited this dispersion relation displays a new branch in the plasmon spectrum.

The purpose of this report is to show that an alternate means of representing the dispersion relation exists, namely as a continued fraction, and that the dispersion relation with a second branch is valid for more general choices of the spatial dependence of the conductivity than that previously studied. In addition, the continued-fraction representation does not necessarily depend upon a local analysis, it readily generates successive orders of approximations to the dispersion relation, and it may possess the rapid convergence which is characteristic of resummation methods.

The technique we propose follows from the observation that the surface-plasmon dispersion is defined by matching a function and its derivative across a discontinuity. By applying a well-known method from the theory of ordinary differential equations, a continued-fraction representation may be established for the ratio of the solution to its derivative.

II. BACKGROUND

Using Ince's notation[6] a general linear second-order differential equation,

$$y''(z)+p(z)y'(z)+q(z)y(z)=0 , \qquad (1)$$

may obviously be reexpressed in the form

$$y(z)=Q_0(z)y'(z)+P_1(z)y''(z) \qquad (2)$$

for nonvanishing $p(z)$ and $q(z)$. Differentiating (2) once and solving for $y'(z)$ yields

$$y'(z)=\left[\frac{Q_0(z)+P_1'(z)}{1-Q_0'(z)}\right]y''(z)+\left[\frac{P_1(z)}{1-Q_0'(z)}\right]y''(z) . \qquad (3)$$

In general, the recursion relation for the derivatives of $y(z)$ is

$$y^{(n)}(z)=Q_n(z)y^{(n+1)}(z)+P_{n+1}(z)y^{(n+2)}(z) , \qquad (4a)$$

where

$$Q_n(z)=\frac{Q_{n-1}(z)+P_n'(z)}{1-Q_{n-1}'(z)} , \qquad P_{n+1}(z)=\frac{P_n(z)}{1-Q_{n-1}'(z)} \qquad (4b)$$

for integral n. To generate a continued-fraction representation for the ratio of the function to its derivative, rearrange Eq. (2) by dividing $y'(z)$ through:

$$\frac{y(z)}{y'(z)}=Q_0(z)+P_1(z)\frac{y''(z)}{y'(z)} . \qquad (5)$$

Clearly, the solution $y(z)$ is related to its derivative by ratios of higher derivatives. Using the recursion relation for the derivative, this process may be continued. That is, (3) may be used to form y'/y''

$$\frac{y'(z)}{y''(z)}=Q_1(z)+P_2(z)\frac{y'''(z)}{y''(z)} , \qquad (6)$$

which is then substituted into (5) to give

$$\frac{y(z)}{y'(z)}=Q_0(z)+\frac{P_1(z)}{Q_1(z)+P_2(z)}\frac{y''(z)}{y'''(z)} .$$

This process, which may be continued to any order by use of (4a) and (4b), generates the desired continued-fraction representation for the quantity y/y'. The convergence criteria for the nonterminating case are given by Ince.[6]

III. APPLICATION TO THE SURFACE-PLASMON DISPERSION RELATION

The prescription for finding electromagnetic surface modes follows from matching conditions on the y component of the magnetic field H_y and the x component of the electric field E_x across an inhomogeneous dielectric layer at the boundary $z=0$.[3] Specifically, $H_y(z)$ is given by the linear second-order differential equation

$$H_y'' - \frac{\epsilon'(z,\omega)}{\epsilon(z,\omega)}H_y'(z)-K^2(z)H_y(z)=0 , \qquad (7)$$

and $E_x(z)$ is expressed in terms of the derivative of $H_y(z)$,

$$E_x(z)=\left[\frac{-i\epsilon}{\omega\epsilon(z,\omega)}\right]H_y'(z) . \qquad (8)$$

The dielectric function $E(z,\omega)$ will be different for $z<0$ and $z>0$. These functions will be designated as $E^{\rm I}(z,\omega)$ and $E^{\rm II}(z,\omega)$, respectively, as will the solutions $H_y^{\rm II}(z)$, $E_x^{\rm II}(z)$, $H_y^{\rm I}(z)$, and $E_x^{\rm I}(z)$. The matching conditions become

$$H_y^{\rm I}(0)=H_y^{\rm II}(0), \quad E_x^{\rm I}(0)=E_x^{\rm II}(0) \qquad (9)$$

or, combining these conditions,

$$\frac{1}{\epsilon^{\rm I}(0)}\frac{H_y^{\rm I}(0)}{(H_y^{\rm I})'(0)}=\frac{1}{\epsilon^{\rm II}(0)}\frac{H_y^{\rm II}(0)}{(H_y^{\rm II})'(0)} . \qquad (10)$$

So, by finding the ratio $H_y(z)/H_y'(z)$ and matching at $z=0$, the dispersion realtion is readily expressed by the continued-fraction technique of Sec. II.

Before proceeding with this construction, it is convenient to rewrite the basic differential equation (7) by separating out the constant term in the dielectric function. Since $K^2(z)$ has the form

$$K_j^2(z)=k_j^2(z)-\alpha_j\epsilon^j(z,\omega), \quad j={\rm I,II}$$

the required separation is

$$K_j^2(z)=k_j^{(2)}(z)+g_j(z,\omega) . \qquad (11)$$

With this notation, the differential equation (7) has the form

$$(H_y^j)''(z)-\frac{(\epsilon^j)'(z,\omega)}{\epsilon^j(z,\omega)}(H_y^j)'(z)-k_j^2(H_y^j)(z)-g_j(z,\omega)(H_y^j)(z)=0 \quad (12)$$

on either side of the inhomogeneity. Now apply the transformation $H_y^j(z)=e^{-k_jz}u_j(z)$ so that (12) becomes

$$u_j''(z)-\left[2k_j+\frac{(\epsilon^j)'(z,\omega)}{\epsilon^j(z,\omega)}\right]u_j'(z)+\left[\frac{(\epsilon^j)'(z,\omega)}{\epsilon^j(z,\omega)}k_j-g_j(z,\omega)\right]u_j(z)=0\,. \quad (13)$$

At this point, the continued fraction may be constructed by manipulating into the form

$$\left[g_j(z,\omega)-\frac{(\epsilon^j)'(z,\omega)}{\epsilon^j(z,\omega)}k_j\right]^{-1}u_j'(z)+\left[2k_j+\frac{(\epsilon^j)'(z,\omega)}{\epsilon^j(z,\omega)}\right]\{[(\epsilon^j)'(z,\omega 0/\epsilon^j(z,\omega)^{k_j-g_j(z,\omega)}]u_j'(z)\}^{-1}=u_j(z)\,. \quad (14)$$

In terms of the function $u_j(z)$, the matching condition (10) becomes

$$\frac{1}{\epsilon^{\mathrm{I}}(0,\omega)}\frac{u_{\mathrm{I}}'(0)}{u_{\mathrm{I}}(0)}-\frac{k_{\mathrm{I}}}{\epsilon^{\mathrm{I}}(0,\omega)}=\frac{1}{\epsilon^{\mathrm{II}}(0,\omega)}\frac{u_{\mathrm{II}}'(0)}{u_{\mathrm{II}}(0)}-\frac{k_{\mathrm{II}}}{\epsilon^{\mathrm{II}}(0,\omega)}\,, \quad (15a)$$

where the continued-fraction representation for $u'(z)/u(z)$ is given entirely in terms of the coefficients of the differential equation. Specializing this result to lowest order, we find

$$\frac{1}{\epsilon^{\mathrm{II}}(0,\omega)}\left[\frac{(\epsilon^{\mathrm{I}})'(0,\omega)}{\epsilon^{\mathrm{I}}(0,\omega)}\right]\Big/\left[2k_{\mathrm{I}}+\frac{(\epsilon^{\mathrm{I}})'(0,\omega)}{\epsilon^{\mathrm{I}}(0,\omega)}\right]-\frac{k_{\mathrm{I}}}{\epsilon^{\mathrm{I}}(0,\omega)}$$
$$=\frac{1}{\epsilon^{\mathrm{II}}(0,\omega)}\left[\frac{(\epsilon^{\mathrm{II}})'(0,\omega)}{\epsilon^{\mathrm{II}}(0,\omega)}k_{\mathrm{II}}\right]\Big/\left[2k_{\mathrm{II}}+\frac{(\epsilon^{\mathrm{II}})'(0,\omega)}{\epsilon^{\mathrm{II}}(0,\omega)}\right]-\frac{k_{\mathrm{II}}}{\epsilon^{\mathrm{II}}(0,\omega)}\,. \quad (15b)$$

Thus, a general dispersion relation is obtained in continued-fraction form.

As a specific application of this result, the lowest-order behavior of the given differential equation which contains the specific choice of dielectric fucntion

$$\epsilon^{\mathrm{II}}(z,\omega)=b(\omega)+s(\omega)e^{-z/a}$$

will be rederived. In this case the field equation for $z>0$ becomes[3,7,8]

$$\eta(\eta+1)u''(\eta)+(2\alpha\eta-1)u'(\eta)-(\alpha+q\eta)u(\eta)=0\,, \quad (16)$$

where $\eta=s/be^{-z/a}-1$ and the parameters α, q, s, and b are chosen to describe the physical system. Equation (16) holds in the region $z>0$; in the region $z<0$, $(\epsilon^{\mathrm{I}})'(z)=0$ and the field equation correspondingly simplifies. The general equation reduces to

$$(H_y^{\mathrm{I}})''(z)+k_{\mathrm{I}}^2H_y^{\mathrm{I}}(z)=0\,,$$

which is trivially solved so that only (16) need be considered. Now, to lowest order in the continued fraction,

$$Q_0(\eta)=Q_0(\eta)=\frac{2\alpha y-1}{\alpha+q\eta}$$

in the notation given above. Thus

$$\left.\frac{u'(\eta)}{u(\eta)}\right|_0\simeq\left.\frac{1}{Q_0(\eta)}\right|_0=-\alpha\,.$$

However, from the power-series analysis[7,8] of the solution of (16),

$$u(\eta)\cong\frac{2}{q+\alpha^2}-\frac{2\alpha}{q+\alpha^2}\eta\,,$$

so that

$$\left.\frac{u'(\eta)}{u(\eta)}\right|_0 = -\alpha ,$$

and the dispersion relation obtained is identical to that found earlier.

IV. DISCUSSION

Several comments should be made about the general dispersion relation (15a). From the method of derivation, it is clear that an arbitrary $\epsilon(z,\omega)$ may be used for modeling a physical system, provided the convergence criteria for the continued fraction are met. Even failing to fulfill these conditions, however, may not necessarily lead to disaster, since the continued fraction may still provide a useful asymptotic resummation which is an accurate representation of the dispersion in the surface excitations. In other words, the continued-fraction representation removes the previous arbitrariness in the choice of dielectric function. This is an important consequence of our analysis, since the method used by Guidotti, Lemberg, and Rice depends on the explicit characteristics of the exponential form of $\epsilon(z)$.

Also, the usual power-series expansion technique for solution of the differential equation has been compressed, in this case, into the convenient form above which will be more generally valid. That is, the form derived above will be valid even in those instances when the power-series expansion of the solution may be slowly converging; such as when $z=0$ is not close to one of the singularities of the general differential equation. Finally, it is obvious that systematic improvement in the orders of expansion is straightforward if a more accurate dispersion relation then (15b) is desired.

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