tions in finite crystalline systems.

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Electrostatic Edge Modes in a Dielectric Wedge

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The dispersion relations are obtained for electrostatic modes localized in the vicinity of the edge of a dielectric wedge formed by the intersection of two semi-infinite planes making an interior angle of 2α. The dielectric constant of the medium is assumed to be isotropic. The resulting modes can be classified as even or odd under reflection in the plane bisecting the wedge. Their frequencies are functions of one continuously varying quantum number. The general results obtained are specialized to yield the dispersion relations for edge optical modes and edge plasmons. Properties of dielectric edge modes are compared and contrasted with corresponding properties of surface modes.

It is well known[1] that at the plane interface between a dielectric medium and the vacuum it is possible for electromagnetic excitations to exist which, while wavelike in directions parallel to the interface, decay exponentially in amplitude with increasing distance from the interface both into the medium and into the vacuum. Such surface excitations have recently been the objects of experimental study.[2]

In this paper we investigate a related problem, namely, electromagnetic excitations localized at the edge of a dielectric wedge whose boundary is formed by the intersection of two semi-infinite planes making an interior angle of 2α. The modes we study are wavelike in the direction parallel to the edge of the wedge, and decay in amplitude with increasing radial distance from the edge and with increasing distance from the two dielectric-vacuum interfaces both into the medium and into the vacuum. We work in the electrostatic limit in the present paper, and obtain expressions for the electrostatic potential describing these excitations as well as their dispersion relations. The nature of these edge excitations when the retardation of the Coulomb interaction is taken into account will be discussed in a subsequent paper.

In a recent paper[3] the dispersion relation and displacement field for vibrational modes localized at the edge of a right-angle wedge of an elastic material have been determined.

We consider a dielectric wedge filling the space $r>0$, $0<\theta<2\alpha$ $(\alpha<\pi)$, and $-\infty<z<\infty$ (see Fig. 1), and characterized by an isotropic dielectric constant $\epsilon(\omega)$. The complementary space, which we will call the vacuum, is characterized by a dielectric constant of unity. The magnetic permeability is assumed to be unity everywhere.

In the electrostatic approximation we must solve for the potential function $\varphi(r, \theta, z)$ which satisfies Laplace's equation

$$\nabla^2\varphi=0 \ . \tag{1}$$

Considerations of infinitesimal translational invariance require that we choose for φ an expression of the form

$$\varphi(r, \theta, z)=f(r, \theta)\, e^{iqz} \ , \tag{2}$$

where $f(r, \theta)$ is a solution of the equation

$$\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\,\frac{\partial}{\partial r}+\frac{1}{r^2}\,\frac{\partial^2}{\partial\theta^2}-q^2\right) f(r, \theta)=0 \ . \tag{3}$$

We separate variables by setting

$$f(r, \theta)=R(r)\,\Theta(\theta) \tag{4}$$

and obtain the pair of equations

$$\frac{d^2}{dr^2}R+\frac{1}{r}\frac{d}{dr}R-\left(q^2-\frac{\mu^2}{r^2}\right)R=0 \ , \tag{5}$$

$$\frac{d^2}{d\theta^2}\Theta=\mu^2\Theta \ , \tag{6}$$

where μ is the separation constant.

The solution of Eq. (5) which decreases with increasing r is

$$R(r)=K_{i\mu}(qr) \ , \tag{7}$$

where $K_{i\mu}(z)$ is the modified Bessel function of the second kind with pure imaginary order. It has the integral representation[4]

$$K_{i\mu}(z)=\int_0^\infty e^{-z\cosh x}\cos\mu x\; dx \ . \tag{8}$$

It is real for μ real and z real and positive, and is an even function of μ. For fixed μ and large z it has the asymptotic form

$$K_{i\mu}(z)\sim\left(\frac{\pi}{2z}\right)^{1/2} e^{-z-\mu^2/2z} \ . \tag{9}$$

The solution of Eq. (6) can be written

$$\Theta(\theta)=a\cosh\mu\theta+b\sinh\mu\theta \ . \tag{10}$$

Because the system being studied has reflection symmetry about the planes $\theta=\alpha$ and $\theta=\alpha+\pi$, we can choose our solutions to be even or odd about these planes. Thus we pick the coefficients a and b in Eq. (10) in such a way that $\Theta(\theta)$ is given by

$$\begin{aligned}\Theta^{(e)}(\theta)&=\cosh\mu(\theta-\alpha)\ , && 0<\theta<2\alpha\\ &=\cosh\mu(\theta-\alpha-\pi)\ , && 2\alpha<\theta<2\pi\end{aligned} \tag{11}$$

$$\begin{aligned}\Theta^{(o)}(\theta)&=\sinh\mu(\theta-\alpha)\ , && 0<\theta<2\alpha\\ &=\sinh\mu(\theta-\alpha-\pi)\ , && 2\alpha<\theta<2\pi\ .\end{aligned} \tag{12}$$

Thus, finally, the electrostatic potential $\varphi(r, \theta, z)$ associated with the dielectric wedge is given by

$$\begin{aligned}\varphi^{(e)}(r, \theta, z)&=AK_{i\mu}(qr)\cosh\mu(\theta-\alpha)\,e^{iqz}\ , \quad 0<\theta<2\alpha\\ &=BK_{i\mu}(qr)\cosh\mu(\theta-\alpha-\pi)\,e^{iqz}\ , \quad 2\alpha<\theta<2\pi\end{aligned} \tag{13}$$

$$\begin{aligned}\varphi^{(o)}(r, \theta, z)&=CK_{i\mu}(qr)\sinh\mu(\theta-\alpha)\,e^{iqz}\ , \quad 0<\theta<2\alpha\\ &=DK_{i\mu}(qr)\sinh\mu(\theta-\alpha-\pi)e^{iqz}\ , \quad 2\alpha<\theta<2\pi\ .\end{aligned} \tag{14}$$

The results given by Eqs. (13) and (14) explain the choice for the sign of the square of the separation constant made in writing Eqs. (5) and (6). Had the opposite choice of sign been made, the radial function $R(r)$ would have been $K_\mu(qr)$, the ordinary

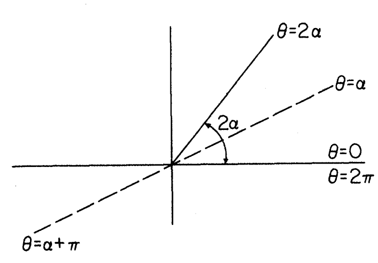

FIG. 1. A dielectric wedge filling the space $r>0$, $0<\theta<2\alpha$ and $-\infty<z<\infty$ and characterized by an isotropic dielectric constant $\epsilon(\omega)$. The complementary space is characterized by a dielectric constant of unity.

modified Bessel function which decreases with increasing argument. The angular function $\Theta(\theta)$, however, would be of the form $a\cos\mu\theta + b\sin\mu\theta$, or oscillatory. With the choice of the sign of μ^2 made here, which leads to Eqs. (13) and (14), we obtain solutions for the potential which, in addition to decreasing with increasing r, decrease exponentially in the directions normal to the planes $\theta = 0$ and $\theta = 2\alpha$, both into the dielectric wedge and into the vacuum outside.

The coefficients A, B, C, D, in Eqs. (13) and (14) have to be determined from the boundary conditions, to which we now turn.

The boundary conditions which must be satisfied are the continuity of the tangential components of the electric field (E_r, E_z) and the normal component of the displacement (D_θ) across the planes $\theta = 0$ and $\theta = 2\alpha$. In fact, because of the way in which we have chosen the angular functions $\Theta^{(e,o)}(\theta)$, it is necessary to satisfy the boundary conditions explicitly only at the plane $\theta = 2\alpha$: Their satisfaction at the plane $\theta = 0$ is then automatic.

The components of the electric field are given by

$$E_r(r, \theta, z) = -\frac{\partial\varphi}{\partial r} , \tag{15a}$$

$$E_\theta(r, \theta, z) = -\frac{1}{r}\frac{\partial\varphi}{\partial\theta} , \tag{15b}$$

$$E_z(r, \theta, z) = -\frac{\partial\varphi}{\partial z} . \tag{15c}$$

From these expressions it follows that the continuity of E_r and E_z at the plane $\theta = 2\alpha$ is ensured if the potential $\varphi(r, \theta, z)$ is continuous across this plane. This condition requires that

$$B = A\,\frac{\cosh\mu\alpha}{\cosh\mu(\pi-\alpha)} , \tag{16a}$$

$$D = -C\,\frac{\sinh\mu\alpha}{\sinh\mu(\pi-\alpha)} . \tag{16b}$$

For the even modes the continuity of D_θ across the plane $\theta = 2\alpha$ yields the condition that

$$B = -A\,\epsilon(\omega)\,\frac{\sinh\mu\alpha}{\sinh\mu(\pi-\alpha)} ; \tag{17a}$$

for the odd modes we obtain the condition

$$D = C\,\epsilon(\omega)\,\frac{\cosh\mu\alpha}{\cosh\mu(\pi-\alpha)} . \tag{17b}$$

Combining Eqs. (16a) and (17a) we obtain the dispersion relation for the even modes

$$\epsilon(\omega) = -\frac{\tanh\mu(\pi-\alpha)}{\tanh\mu\alpha} \quad \text{(even)} . \tag{18}$$

The dispersion relation for the odd modes, which follows from combining Eqs. (16b) and (17b) is

$$\epsilon(\omega) = -\frac{\tanh\mu\alpha}{\tanh\mu(\pi-\alpha)} \quad \text{(odd)} . \tag{19}$$

We apply the results represented by Eqs. (18) and (19) to two cases of physical interest. The first is a dielectric wedge constructed from a diatomic cubic ionic crystal or polar semiconductor, whose dielectric constant is given by

$$\epsilon(\omega) = \epsilon_\infty\,\frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2} . \tag{20}$$

In this expression ϵ_∞ is the optical frequency dielectric constant, and ω_L and ω_T are the frequencies of the longitudinal- and transverse-optical vibration modes of infinite wavelength. When Eq. (20) is substituted into Eqs. (18) and (19), and the resulting equations are solved for ω, the results are

$$\omega = \left(\frac{\epsilon_0 + x}{\epsilon_\infty + x}\right)^{1/2} \omega_T \quad \text{(even)} \tag{21}$$

for the even modes, and

$$\omega = \left(\frac{x\epsilon_0 + 1}{x\epsilon_\infty + 1}\right)^{1/2} \omega_T \quad \text{(odd)} \tag{22}$$

for the odd modes. To simplify these expressions we have set

$$x = \frac{\tanh\mu(\pi-\alpha)}{\tanh\mu\alpha} , \tag{23}$$

and ϵ_0 is the static dielectric constant, which enters the theory through the Lyddane–Sachs–Teller relation, $\epsilon_\infty\omega_L^2 = \epsilon_0\,\omega_T^2$. The dispersion curves for edge optical modes given by Eqs. (21)–(23) are plotted for wedges of GaP defined by $\alpha = \pi/8$, $\pi/4$, and $3\pi/8$ in Fig. 2.

The second case we consider is that of a wedge of an n-type semiconductor, whose dielectric constant is given by

$$\epsilon(\omega) = \epsilon_\infty\,(1 - \omega_p^2/\omega^2) , \tag{24}$$

where ω_p is the plasma frequency of the free carriers in the semiconductor, and is defined by

$$\omega_p^2 = 4\pi n e^2/m^*\,\epsilon_\infty . \tag{25}$$

In Eq. (25) n is the density of free carriers and m^* is the effective mass of each. In this case ϵ_∞ plays the role of the background dielectric constant of the semiconductor. When Eq. (24) is substituted into Eqs. (18) and (19), the solutions can be written as

$$\omega = \left(\frac{\epsilon_\infty}{\epsilon_\infty + x}\right)^{1/2} \omega_p \quad \text{(even)} \tag{26}$$

for the even modes, and

$$\omega = \left(\frac{\epsilon_\infty x}{\epsilon_\infty x + 1}\right)^{1/2} \omega_p \quad \text{(odd)} \tag{27}$$

for the odd modes. The frequencies of edge plasmons given by Eqs. (26) and (27) are plotted for

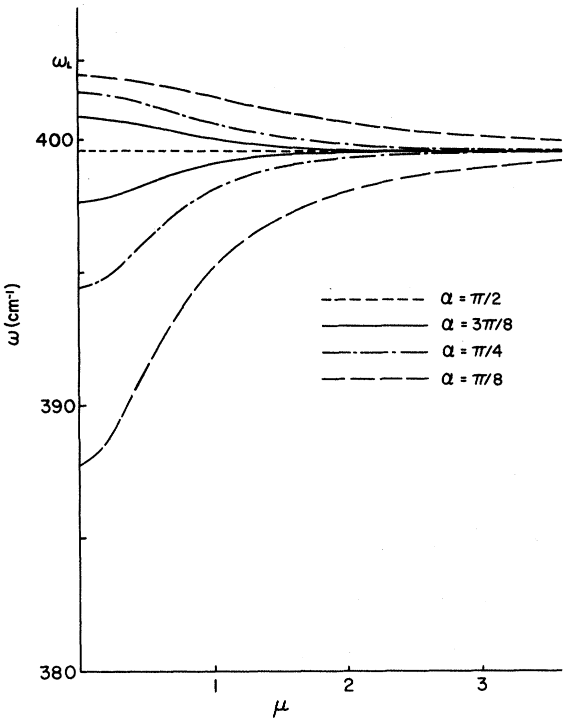

FIG. 2. Dispersion curves for edge optical modes of GaP plotted for different values of α (2α is the wedge angle). The odd modes lie above the dispersion curve for $\alpha = \pi/2$ and the even modes below. The following data were used for GaP: $\omega_T = 367.3$ cm^{-1}; $\omega_L = 403.0$ cm^{-1}; $\epsilon_\infty = 9.091$; and $\epsilon_0 = 10.944$.

wedges of n-type InSb defined by $\alpha = \pi/8$, $\pi/4$, and $3\pi/8$ in Fig. 3.

From the results presented in Figs. 2 and 3 we see that in general the frequencies of the even modes are lower than the frequencies of the odd modes for all values of $\mu > 0$, provided that $\alpha < \pi/2$. For angles $\alpha > \pi/2$, the reverse is true. From Eqs. (18) and (19) we see that the even modes for a wedge angle $\alpha > \pi/2$ have the same dispersion relation as do the odd modes for a wedge angle of $\pi - \alpha$, while the odd modes for a wedge angle $\alpha > \pi/2$ have the same dispersion relation as the even modes for a wedge angle of $\pi - \alpha$.

For the special value of $\alpha = \pi/2$ the dispersion relations for the even and odd modes coincide, and are independent of μ. Since this special value of α corresponds to the case that the wedge opens up to fill the upper half space $r > 0$, $0 < \theta < \pi$, $-\infty < z < \infty$, with a plane dielectric-vacuum interface it is interesting to compare and contrast the preceding results with the corresponding results for surface modes on a dielectric medium filling a half-space. Although the results in this case are well known,[1] we rederive them here in a way designed to facilitate this comparison. Accordingly, we consider the system depicted in Fig. 4. A dielectric medium characterized by a dielectric constant $\epsilon(\omega)$ occupies the half-space $y > 0$. The half-space $y < 0$ is the vacuum. We seek the potential function $\varphi(x, y, z)$ in the form

$$\varphi(x, y, z) = f(x, y)\, e^{iqz} , \tag{28}$$

so that the function $f(x, y)$ satisfies the equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - q^2\right) f(x, y) = 0 . \tag{29}$$

We separate variables by putting

$$f(x, y) = Y(X)\, Y(y) , \tag{30}$$

and obtain the pair of equations

$$\frac{d^2}{dx^2} X = -\nu^2 X , \tag{31}$$

$$\frac{d^2}{dy^2} Y = (q^2 + \nu^2) Y , \tag{32}$$

where ν is the separation constant. The choice of sign for ν^2 on the right-hand sides of Eqs. (31) and (32) is dictated both by the invariance of the system against infinitesimal displacements in the x direction, and by our requirement that the poten-

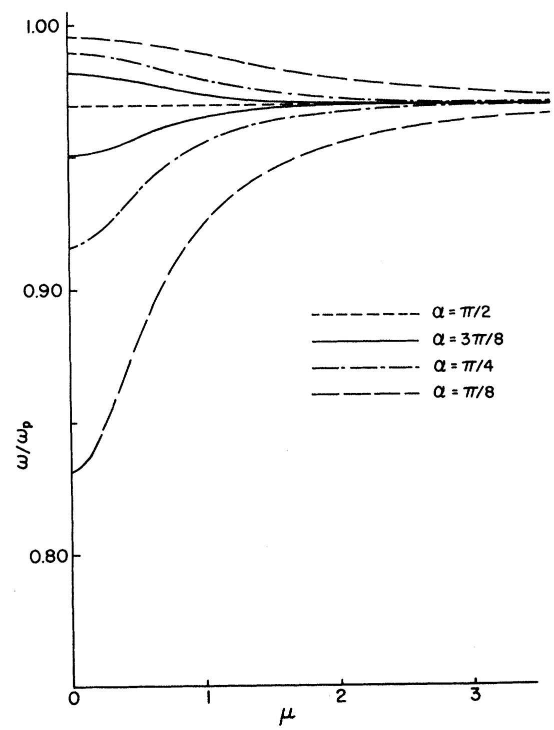

FIG. 3. Dispersion curves for edge plasmons in n-type InSb plotted for different values of the wedge angle 2α. The odd modes lie above the dispersion curve for $\alpha = \pi/2$ and the even modes below. The experimental result for ϵ_∞ was taken to be $\epsilon_\infty = 15.68$.

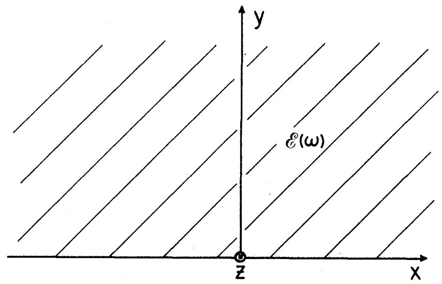

FIG. 4. A dielectric medium filling the half-space $y>0$ and characterized by an isotropic dielectric constant $\epsilon(\omega)$. The complementary half-space is characterized by a dielectric constant of unity.

tial decreases to zero with increasing distance from the surface into the medium and into the vacuum.

The solution of Eq. (31) can be written in the form

$$X(x)=a\cos\nu x+b\sin\nu x\ , \tag{33}$$

while the solution of Eq. (32) with the required property is

$$\begin{aligned} Y(y)&=e^{-(q^2+\nu^2)^{1/2}y}\ , \qquad y>0\\ &=e^{(q^2+\nu^2)^{1/2}y}\ , \qquad y<0\ . \end{aligned} \tag{34}$$

With no loss of generality we can divide our solutions into those which are even under reflection in the yz plane and those that are odd. Consequently, we obtain for $\varphi(x,y,z)$ the results

$$\varphi^{(e)}(x,y,z)=A\cos\nu x\, e^{-(q^2+\nu^2)^{1/2}|y|}\, e^{iqz}\ , \tag{35a}$$

$$\varphi^{(o)}(x,y,z)=B\sin\nu x\, e^{-(q^2+\nu^2)^{1/2}|y|}\, e^{iqz}\ . \tag{35b}$$

By writing the potential in a form which is continuous across the plane $y=0$ we have assured the continuity of the tangential components of $\vec{E}(E_x, E_z)$ across this plane. The continuity of the normal component of $\vec{D}$ across the plane $y=0$ yields the same dispersion relation,

$$\epsilon(\omega)=-1\ , \tag{36}$$

for both the even and the odd modes.

From the preceding analysis we see that for both edge modes and surface modes the separation constant (μ for edge modes, ν for surface modes) plays the role of one of the two continuously varying quantum numbers (the second being q) characterizing the potential and hence the electrostatic fields of the modes. However, the edge modes differ from the surface modes in that their dispersion relations are functions of the continuously varying quantum number which is the separation constant μ, although they are independent of the quantum number q, while the dispersion relation (36) for surface modes is independent of both continuously varying quantum numbers ν and q. In the limit as $\mu\to\infty$, however, we see from Eqs. (18) and (19) that the dispersion relations for the even and odd edge modes both approach the dispersion relation (36) for surface modes. The frequencies given by combining Eqs. (36) with Eqs. (20) and (24) are plotted as dashed lines in Figs. 2 and 3, respectively. It should also be noted that the dispersion relation for surface modes, Eq. (36), is just that for the even and odd edge modes, Eqs. (18) and (19), for all values of μ in the special case $\alpha=\pi/2$, when the wedge fills the upper half space.

Just as the dispersion relation for dielectric surface excitations becomes a function of q when retardation is taken into account,[5] we expect that the dispersion relation for edge modes will become a function of both μ and q in the same limit.

An interesting limiting case of Eqs. (13), (14), and (16) is that for $\alpha=\pi/2$. In this case the dielectric wedge fills the upper half space $r>0$, $0<\theta<\pi$, $-\infty<z<\infty$, which is the situation assumed in our discussion of surface waves. The potential functions $\varphi^{(e)}(r,\theta,z)$ and $\varphi^{(o)}(r,\theta,z)$ in this case take the forms

$$\begin{aligned} \varphi^{(e)}(r,\theta,z)&=AK_{i\mu}(qr)\cosh\mu(\theta-\pi/2)\,e^{iqz}\ , \quad 0<\theta<\pi\\ &=AK_{i\mu}(qr)\cosh\mu(\theta-3\pi/2)\,e^{iqz}\ , \quad \pi<\theta<2\pi \end{aligned} \tag{37a}$$

$$\begin{aligned} \varphi^{(o)}(r,\theta,z)&=CK_{i\mu}(qr)\sinh\mu(\theta-\pi/2)\,e^{iqz}\ , \quad 0<\theta<\pi\\ &=CK_{i\mu}(qr)\sinh\mu(\theta-3\pi/2)\,e^{iqz}\ , \quad \pi<\theta<2\pi\ . \end{aligned} \tag{37b}$$

Because the physical configurations are the same, and because the frequencies of the two kinds of modes are the same, the question arises as to whether it is possible to superpose the wavelike surface modes given by Eq. (35), which decay only in the directions normal to the dielectric-vacuum interface, in such a way as to obtain the edge modes described by Eq. (37), which decay not only with increasing r but also with increasing θ as one goes away from the interface. In other words, is it possible to find functions $g_\mu(\nu)$ and $h_\mu(\nu)$, independent of x and y, such that, for example, the relations

$$\int_0^\infty g_\mu(\nu)\cos\nu x\, e^{-(q^2+\nu^2)^{1/2}y}\,d\nu=K_{i\mu}(qr)\cosh\mu(\theta-\pi/2) \tag{38a}$$

and

$$\int_0^\infty h_\mu(\nu)\sin\nu x\, e^{-(q^2+\nu^2)^{1/2}y}\,d\nu=K_{i\mu}(qr)\sinh\mu(\theta-\pi/2) \tag{38b}$$

are satisfied for $-\infty<x<\infty$, $y>0$ and $r>0$, $0<\theta<\pi$? The answer is yes, and requires for its demonstration the following two integrals[6]:

$$\int_0^\infty d\nu \, \frac{1}{2(q^2+\nu^2)^{1/2}} \left[\left(\frac{(q^2+\nu^2)^{1/2}+\nu}{q} \right)^{i\mu} + \left(\frac{(q^2+\nu^2)^{1/2}-\nu}{q} \right)^{i\mu} \right] \cos\nu x \, e^{-(q^2+\nu^2)^{1/2}y}$$
$$= K_{i\mu}[q(x^2+y^2)^{1/2}] \cosh\mu\left(\frac{\pi}{2} - \tan^{-1}\frac{y}{x} \right) , \quad (39a)$$

$$\int_0^\infty d\nu \, \frac{1}{2i(q^2+\nu^2)^{1/2}} \left[\left(\frac{(q^2+\nu^2)^{1/2}-\nu}{q} \right)^{i\mu} - \left(\frac{(q^2+\nu^2)^{1/2}+\nu}{q} \right)^{i\mu} \right] \sin\nu x \, e^{-(q^2+\nu^2)^{1/2}y}$$
$$= K_{i\mu}[q(x^2+y^2)^{1/2}] \sinh\mu\left(\tan^{-1}\frac{y}{x} - \frac{\pi}{2} \right) , \quad (39b)$$

where the branch cut for the arctangent is along the negative real axis ($x<0$, $y=0$). Comparing Eqs. (38) and (39) we see that the functions $g_\mu(\nu)$ and $h_\mu(\nu)$ are given by

$$g_\mu(\nu) = \frac{1}{(q^2+\nu^2)^{1/2}} \cos\left(\mu \ln \frac{(q^2+\nu^2)^{1/2}+\nu}{q} \right) , \quad (40a)$$

$$h_\mu(\nu) = \frac{-1}{(q^2+\nu^2)^{1/2}} \sin\left(\mu \ln \frac{(q^2+\nu^2)^{1/2}+\nu}{q} \right) . \quad (40b)$$

Analogous results can be obtained relating the potentials (35) and (37) for $y<0$ or $\pi<\theta<2\pi$, i.e., in the vacuum.

Thus, we have demonstrated the existence of dielectric edge modes in the electrostatic approximation, have obtained the potential function from which their electric fields are derived, have obtained their dispersion relations, have solved them in two particular cases, and have shown them to be a linear superposition of dielectric surface modes of the same frequency in the special case that the dielectric wedge fills the upper half space, the only case in which such a superposition can be made.

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[1]For a review of various kinds of surface excitations the reader is referred to the articles by R. F. Wallis [in *Enrico Fermi Summer School on Atomic Structure and Properties of Solids*, *Varenna*, *Italy*, 1971 (Academic, New York, to be published)] and by T. Wolfram [J. Vac. Sci. Technol. (to be published)].

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[4]See, for example, F. Oberhettinger, *Tabellen zur Fourier Transformation* (Springer-Verlag, Berlin, 1957), p. 40.

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[6]These integrals are obtained from results given in Ref. 4, pp. 14 and 125, respectively.