Electrostatic edge modes of a dielectric wedge

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The calculation of the electrostatic edge modes of a dielectric wedge by Dobrzynski and Maradudin is reconsidered. It is shown that the electric fields are singular and the field energy is infinite near the edge. Rounding the edge by taking the boundary to be a hyperbolic cylinder removes the singularity, but changes the spectrum from continuous and independent of q (where $\phi \propto e^{iqz}$) to discrete and dependent upon q. For the rounded edge these modes possess an orthogonality property convenient for calculating the response of the dielectric to an external charge.

Dobrzynski and Maradudin have calculated the electrostatic edge modes of a dielectric wedge.[1] The boundaries of the wedge were formed by the intersection of two semi-infinite planes making an interior angle 2α. As shown below, the electric fields associated with the edge modes are singular. The singularity is strong enough to make the field energy $(1/8\pi)\int dV|\nabla\phi|^2$ infinite in the neighborhood of the edge. Hence, the fields violate the Meixner criterion[2] and cannot be normalized. If one were to attempt to quantize these edge modes, the infinite field energy would cause difficulty. The singular nature of the fields may also be important in the calculation of the optical reflectivity and absorption of solids with sharp edges.[3,4]

Rounding the edge of the wedge removes the singularity. So in this paper we analyze a particular model of a rounded edge, namely, a dielectric whose boundary is a hyperbolic cylinder (see Fig. 1). The distance from the origin to the focus is a and the eccentricity is $\sec\alpha$. In the limit $a\to 0$, we recover the wedge with the sharp edge.

After a brief statement of the problem for either type of boundary, the solution for the wedge with a sharp edge is reviewed. Next the solution for the rounded edge is given. Lastly, the orthogonality of these solutions is discussed.

Following Dobrzynski and Maradudin,[1] we neglect retardation and nonlocal effects. Then the problem is to find solutions of Laplace's equation $\nabla^2\phi = 0$, for which the potential ϕ and the normal component of the displacement are continuous across the boundary. Also, ϕ must vanish at infinity. Solutions are allowed only for certain, negative values of the dielectric constant ϵ.[5] For example, when $\alpha = \frac{1}{2}\pi$ (flat surface), only $\epsilon = -1$ is allowed (corresponding to the surface plasmon for the case of a metal).

Let us examine the wedge with a sharp edge. In this case cylindrical coordinates (r,θ,z) are convenient with the dielectric occupying $r>0$, $-\alpha<\theta<\alpha$, and $-\infty<z<\infty$.[6] For modes even in θ (i.e., about the midplane of the wedge) the solutions are[1]

$$\phi(r,\theta,z) = AK_{i\mu}(qr)\cosh\mu\theta e^{iqz} \quad (-\alpha<\theta<\alpha) \tag{1a}$$

$$= BK_{i\mu}(qr)\cosh\mu(\pi-\theta)e^{iqz} \quad (\alpha<\theta<2\pi-\alpha), \tag{1b}$$

where

$$B = A\cosh\mu\alpha/\cosh\mu(\pi-\alpha) \tag{1c}$$

and

$$\epsilon = -\tanh\mu(\pi-\alpha)/\tanh\mu\alpha, \quad 0\le\mu<\infty. \tag{1d}$$

A is a constant and $K_{i\mu}(x)$ is a modified Bessel function of the second kind with imaginary order. The odd solutions can be found by replacing cosh by sinh and ϵ by $1/\epsilon$ in Eq. (1). Note that the ω dependence of ϵ is suppressed. In fact, it is convenient to regard ϵ as an eigenvalue.[5] The actual computation of frequencies of oscillation (such as $\omega_p/\sqrt{2}$ for the surface plasmon) can be done straightforwardly by equating $\epsilon(\omega)$ with the allowed values of ϵ. As $x\to 0$, it can be shown that

$$K_{i\mu}(x)\to -(\pi/\mu\sinh\mu)^{1/2} \times \sin[\mu\ln(\tfrac{1}{2}x) - \arg\Gamma(1+i\mu)], \tag{2}$$

which remains finite although it is rapidly oscillating as $x\to 0$. The field $-\nabla\phi$, however, goes as $1/r$ times a rapidly oscillating function ($\sin[\mu\ln(kr)$ + phase angle]). So $|\nabla\phi|^2$ goes essentially as $1/r^2$ and $\int r\,dr|\nabla\phi|^2$ goes as $\ln r$, $r\to 0$. The field energy, therefore, will be infinite unless r is cut off at some nonzero value. The hyperbolic boundary removes the singularity in this way, so we consider it next.

It is convenient to introduce elliptic cylinder coordinates[7]

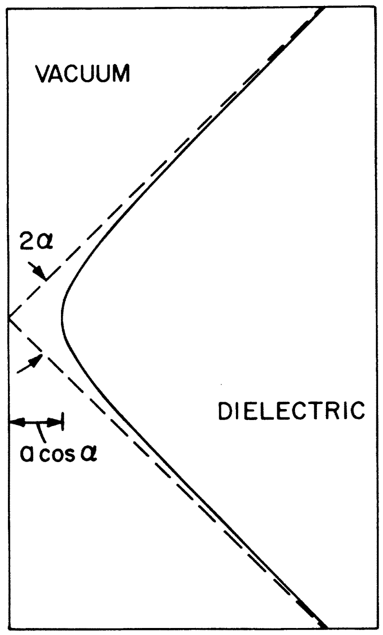

FIG. 1. Cross section of dielectric whose boundary is a hyperbolic cylinder. The z axis is perpendicular to the drawing.

$$x = a\cosh\xi\cos\eta, \quad 0 \le \xi < \infty, \quad -\alpha \le \eta \le 2\pi - \alpha, \tag{3a}$$

$$y = a\sinh\xi\sin\eta, \tag{3b}$$

$$z = z. \tag{3c}$$

The dielectric occupies $\xi \ge 0$, $-\alpha < \eta < \alpha$, and $-\infty < z < \infty$. The vacuum occupies $\xi \ge 0$, $\alpha < \eta < 2\pi - \alpha$, and $-\infty < z < \infty$. The upper-half of the boundary is given by $\eta = \alpha$ and the lower-half by $\eta = -\alpha$ when approached from the dielectric and $\eta = 2\pi - \alpha$ when approached from the vacuum. The gradient of ϕ is given by

$$\mathrm{grad}_\xi\phi = \frac{1}{h(\xi,\eta)}\frac{\partial\phi}{\partial\xi}, \tag{4a}$$

$$\mathrm{grad}_\eta\phi = \frac{1}{h(\xi,\eta)}\frac{\partial\phi}{\partial\eta}, \tag{4b}$$

and

$$\mathrm{grad}_z\phi = \frac{\partial\phi}{\partial z}, \tag{4c}$$

where

$$h(\xi,\eta) = a(\sinh^2\xi + \sin^2\eta)^{1/2}. \tag{4d}$$

Laplace's equation becomes

$$\frac{1}{h^2(\xi,\eta)}\left(\frac{\partial^2\phi}{\partial\xi^2}\right) + \frac{\partial^2\phi}{\partial z^2} = 0. \tag{5}$$

The boundary conditions are that ϕ is continuous across the boundary and that

$$\frac{\partial\phi}{\partial\eta}(\text{vacuum}) = \epsilon\frac{\partial\phi}{\partial\eta}(\text{dielectric})$$

at the boundary. Also $\phi \to 0$ as $\xi \to \infty$.

It is well known that Laplace's equation is separable in this coordinate system, so we write

$$\phi(\xi,\eta,z) = f(\xi)g(\eta)e^{iqz}. \tag{6}$$

Then Eq. (5) implies that

$$\frac{d^2f}{d\xi^2} + (E - q^2a^2\sinh^2\xi)f = 0 \tag{7}$$

and

$$\frac{d^2g}{d\eta^2} - (E + q^2a^2\sin^2\eta)g = 0, \tag{8}$$

where E is the separation parameter.

Each solution will be either even or odd about the midplane. For the even solutions, then both $f(\xi)$ and $g(\eta)$ are even functions; and for the odd solutions, $f(\xi)$ and $g(\eta)$ are odd. In both cases, $f(\xi) \to 0$ as $\xi \to \infty$.

Equation (7) is equivalent to finding the eigenvalues and eigenfunctions of a particle in the potential well $V(\xi) = \text{const}\sinh^2\xi$. Clearly, only discrete, positive values of E are allowed. For example when $q^2a^2 \gg 1$, for the lowest eigenvalues $\sinh^2\xi$ can be replaced by ξ^2 and then the solutions are the harmonic-oscillator solutions with $E = (2n+1)qa$, $n = 0, 1, 2, \ldots$. In general, we must use numerical means to solve (7) although it is clear that we can label the solutions with a discrete index n as in the harmonic-oscillator problem. The solutions will be localized near the edge, mostly within the classical turning point.

The discrete values E_n are then inserted into (8) to determine $g_n(\eta)$, which must also be calculated numerically. For the dielectric we write

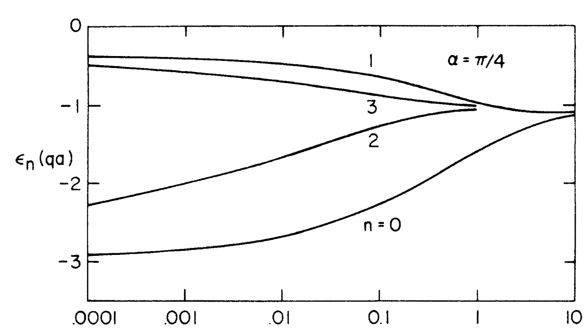

FIG. 2. Allowed values of ϵ vs qa. Only the first four are shown. Higher n values cluster about -1. Even values of n correspond to even modes and odd values to odd modes.

$$\phi(\xi, \eta, z) = A f_n(\xi) g_n(\eta) e^{iqz}, \quad -\alpha < \eta < \alpha, \tag{9}$$

and for the vacuum

$$\phi(\xi, \eta, z) = B f_n(\xi) g_n(\pi - \eta) e^{iqz}, \quad \alpha < \eta < 2\pi - \alpha. \tag{10}$$

Matching ϕ and the normal component of the displacement at the boundary $\eta = \alpha$ gives

$$B = A g_n(\alpha) / g_n(\pi - \alpha) \tag{11a}$$

and

$$\epsilon = -\frac{g_n(\alpha) g_n'(\pi - \alpha)}{g_n'(\alpha) g_n(\pi - \alpha)}. \tag{11b}$$

Nothing additional is gained from the other boundary when the even or odd nature of the solution is taken into account. We see that the allowed values of ϵ are discrete for a given qa. We denote them by $\epsilon_n(qa)$. This is in contrast to Ref. 1 where the allowed values are continuous and independent of q. In Fig. 2 the first four allowed values are plotted as a function of qa for $\alpha = \frac{1}{4}\pi$. We note that as $qa \to \infty$, for all n, $\epsilon_n(qa) \to -1$. This is to be expected physically since curvature becomes less important as the wavelength decreases, thereby approaching the limit of a flat surface.

As $qa \to 0$, the potential well becomes more shallow and the energy levels become closer together. Numerically, this occurs for $qa \lesssim 0.01$ in Fig. 2. In fact at $qa = 0$, the spectrum of ϵ is continuous and is given by the same formulas as found by Dobrzynski and Maradudin [Eq. (1d) of the present paper for even modes] for the wedge with no rounding.

From general considerations similar to those given in Ref. 5, one can show that, independent of the exact shape of the boundary, for any two solutions ϕ_{nq} and $\phi_{n'q'}$,

$$\int d\vec{S} \cdot \nabla \phi_{nq} \phi^*_{n'q'} = \delta_{nn'} \delta(q - q'), \tag{12}$$

where the surface integral is over the boundary and the gradient is evaluated just inside the dielectric.[8] It is clear that the solutions found in this paper satisfy (12). This rather unusual orthogonality condition is useful if one wishes to quantize the modes or to express the response of the dielectric to an external charge in terms of the electrostatic modes (analogous to finding the image force in terms of surface plasmons[9,10]). For the solutions of Ref. 1 for the wedge with no rounding [Eq. (1) of this paper], no such orthogonality condition exists due to the peculiar behavior of the $K_{i\mu}(qr)$ at small r.

The main conclusion from this work is that a slight rounding of the sharp edge of a dielectric has significant effects on the electrostatic modes. Any property which is dependent upon these modes is also affected.

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[1]L. Dobrzynski and A. A. Maradudin, Phys. Rev. B 6, 3810 (1972).

[2]Josef Meixner, IEEE Trans. AP-20, 442 (1972).

[3]D. W. Berreman, Phys. Rev. 163, 855 (1967); Phys. Rev. B 1, 381 (1970); *Localized Excitations in Solids*, edited by R. F. Wallis (Plenum, New York, 1968), p. 420ff.

[4]R. Fuchs, Phys. Rev. B 11, 1732 (1975).

[5]A. P. van Gelder, J. Holvast, J. H. M. Stoelinga, and P. Wyder, J. Phys. C 5, 2757 (1972).

[6]This choice of coordinate system differs by a rotation of α from that of Ref. 1.

[7]W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea, New York, 1949), p. 148.

[8]In Ref. 5, it is shown by a variational procedure that if the potential inside a finite dielectric is expanded in real, harmonic functions, i.e., $\phi(\vec{r}) = \sum_i c_i u_i(\vec{r})$, then the c_i must solve the eigenvalue equation $\underline{S}\vec{c} = 4\pi/(1 - \epsilon)\underline{G}\vec{c}$. The matrices $\underline{S}$ and $\underline{G}$ are Hermitian and are defined by Eqs. (9) and (10) of Ref. 5. For any two solutions $\vec{c}^{(k)}$ and $\vec{c}^{(m)}$, $k \neq m$, it can be shown that $\sum_{i,j} c_i^{(k)} G_{ij} c_j^{(m)} = 0$. Since $G_{ij} = \int u_i \nabla u_j \cdot d\vec{S}$, then $\int \phi_k \nabla \phi_m \cdot d\vec{S} = 0$. Equation (12) follows from a generalization of this result.

[9]A. A. Lucas, Phys. Rev. B 4, 2939 (1971).

[10]R. Ray and G. D. Mahan, Phys. Lett. A 42, 301 (1972).