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Electrostatic edge modes of a hyperbolic dielectric wedge: Analytical solution

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An *analytical* solution to the problem of finding the electrostatic edge eigenmodes of a hyperbolic dielectric wedge is given and compared with the *numerical* solution given by Davis [Phys. Rev. B **14**, 5523 (1976)]. The results presented here reproduce the solutions found when the hyperbolic dielectric wedge tends to a sharp-edged dielectric wedge.

The study of edge modes on dielectric wedges was started by Dobrzynski and Maradudin.[1] These authors modeled sharp-edged wedges of varying apex angle. The wedges were considered to be infinite in the transverse direction. They concluded that the resulting eigenmodes can be classified as even or odd under reflection in the plane bisecting the wedge, and that their frequencies are functions of one continuously varying quantum number (the separation constant in Laplace's equation) and independent of the wave number.

Later studies showed that the above dependence of the eigenfrequencies can be removed by using a hyperbolic cylinder[2] or a parabolic cylinder[3]—a treatment of the retarded edge modes is given by Boardman, Aers, and Teshima[4]—to model the dielectric wedge or, in a somewhat different approach, by considering nonlocal effects in the dielectric function and maintaining the sharp-edged model for the dielectric wedge.[5] In all these cases, the eigenfrequencies were obtained as a function of the wave number and of a discrete quantum number.

However, the method proposed by Davis[2] is not completely satisfactory, because he solves numerically an equation which can be solved *analytically* in terms of Mathieu and related functions. A detailed study of the latter approach allows us to show analytically that the electrostatic potential and the dispersion relation obtained by Dobrzynski and Maradudin[1] can be obtained when the hyperbolic wedge goes to a sharp wedge.

Interest in the theoretical analysis of wedge excitations has recently been renewed due to the improved electron scattering experiments performed by Marks, Cowley, and Wheatley, Howie, and McMullan,[6] who exploited the technique of scanning transmission electron microscopy (STEM) as a tool of material analysis. They measured[6] the spectra of energy losses of well-focused electron beams interacting with small cubic crystallites of nanometer dimensions of various oxides; the problem is to relate the experimental data with the edge modes that the crystallites may sustain. The beam probe can be kept either external or internal to the sample, and in the former case the long-range interaction between the electron beam and the solid is little distorted by bulk effects. Some theoretical analyses are available of the interaction of electron beams with flat[6] or parabolically shaped wedges,[7] but other geometries have yet to be investigated.

The geometry proposed by Davis[2] to solve the problem of finding the electrostatic edge modes on a hyperbolic wedge is depicted in Fig. 1 and is conveniently described in elliptic cylinder coordinates (ξ,η,z) such that[8]

$$\begin{aligned} x &= h\cosh\xi\cos\eta, \quad 0\le\xi<\infty, \quad 0\le\eta\le 2\pi\ , \\ y &= h\sinh\xi\sin\eta\ , \\ z &= z\ . \end{aligned} \tag{1}$$

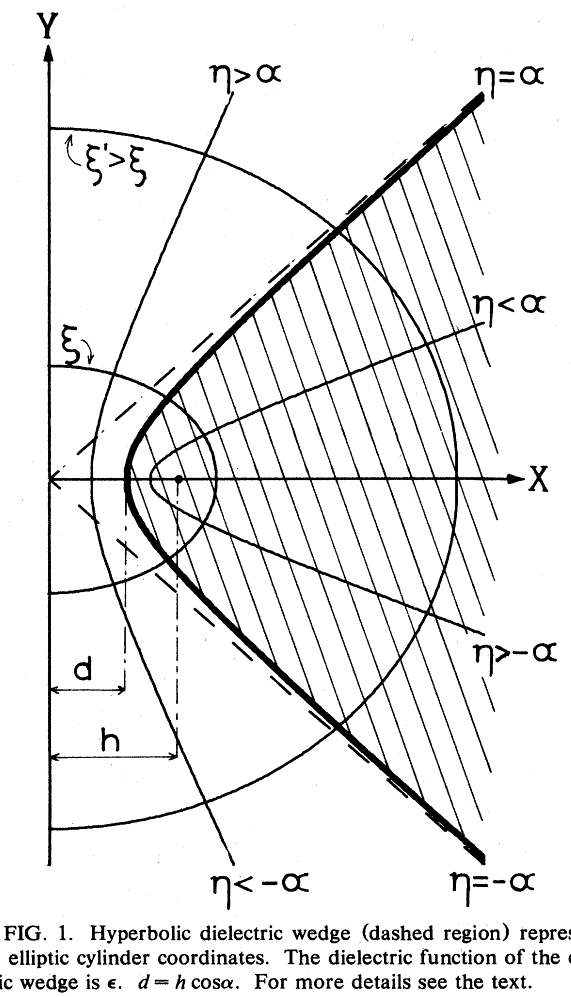

FIG. 1. Hyperbolic dielectric wedge (dashed region) represented in elliptic cylinder coordinates. The dielectric function of the dielectric wedge is ϵ. $d=h\cos\alpha$. For more details see the text.

The point $(\pm h,0)$ represents the common foci of the family of confocal ellipses and of confocal hyperbolas.

The dielectric wedge occupies the region $\xi \geq 0$, $-\alpha \leq \eta \leq \alpha$, and $-\infty < z < \infty$ (z is perpendicular to the xy plane). The vacuum occupies the region $\xi \geq 0$, $\alpha < \eta < 2\pi - \alpha$, and $-\infty < z < \infty$. The upper half of the boundary is given by $\eta = \alpha$, and the lower half is given by $\eta = -\alpha$ when approached from the dielectric, and by $\eta = 2\pi - \alpha$ when approached from the vacuum. The distance to any point (x,y) from the origin, expressed in elliptic cylindrical coordinates, is

$$r = (x^2+y^2)^{1/2} = h[\cosh(2\xi)+\cos(2\eta)]^{1/2}/\sqrt{2} \ . \tag{2}$$

The electrostatic edge modes of the system are obtained by solving Laplace's equation for the potential $\phi(\xi,\eta,z;t)$:

$$\nabla^2\phi(\xi,\eta,z;t) = 0 \ . \tag{3}$$

Because of translational invariance along the z axis we can write

$$\phi(\xi,\eta,z;t) = \phi(\xi,\eta)\exp[i(kz-\omega t)] \ , \tag{4}$$

where k and ω are the wave number and the frequency, respectively, of the electrostatic modes. Then, Eq. (3), in elliptic cylindrical coordinates, becomes

$$\frac{\partial^2\phi(\xi,\eta)}{\partial\xi^2} + \frac{\partial^2\phi(\xi,\eta)}{\partial\eta^2} - k^2h^2(\sinh^2\xi + \sin^2\eta)\phi(\xi,\eta) = 0 \ . \tag{5}$$

The boundary conditions are the continuity of the electrostatic potential and of the normal component of the displacement across the boundary between the vacuum and the dielectric. If the potential due to the edge modes is to be physical, it must vanish when $\xi \to \infty$.

The factorization

$$\phi(\xi,\eta) = f(\xi)g(\eta) \ , \tag{6}$$

allows separation of the variables in Laplace's equation, and Eq. (5) gives

$$\frac{d^2g(\eta)}{d\eta^2} + [-E_n - 2q\cos(2\eta)]g(\eta) = 0 \ , \tag{7}$$

$$\frac{d^2f(\xi)}{d\xi^2} - [-E_n - 2q\cosh(2\xi)]f(\xi) = 0 \ , \tag{8}$$

where

$$q = -\frac{k^2h^2}{4} \ . \tag{9}$$

E_n is the discrete separation constant, which can be obtained as a perturbative solution to the eigenvalues of the harmonic oscillator by considering the series development of $\sinh^2\xi$ for small ξ (close to the edge). Thus, by applying perturbation theory,[9,10] we obtain

$$E_n \cong \frac{k^2h^2}{2} + kh(2n+1) + \tfrac{1}{4}(2n^2+2n+1) + \frac{1}{kh}\frac{1}{180}(20n^3+30n^2+40n+15) + O((kh)^{-2}) \qquad n = 0,1,2,\ \ldots\ , \tag{10}$$

up to first order in perturbation theory. The choice of the sign in the separation constant E_n ensures that the solutions to Eq. (5) are localized at the wedge.

Let us examine the behavior of the differential equations (7) and (8) in the limit $h \to 0$. In this case the hyperbola that defines the wedge tends to the sharp wedge with semiapex angle α. It is easy to prove that, in this case, η tends to the polar angular coordinate θ, and ξ is related to the polar radial coordinate r through expression (2). When $h \to 0$, Eq. (7) [Eq. (8)] becomes exactly the differential equation for the angular (radial) component of the electrostatic potential in the case of a sharp-edged dielectric wedge, i.e., Eq. (6) [Eq. (5)] in the paper of Dobrzynski and Maradudin.[1]

Although solutions to Eqs. (7) and (8) are, respectively, Mathieu and modified Mathieu functions, we will express our solutions to these equations in a manner which reproduces, naturally, the solutions found by Dobrzynski and Maradudin[1] for the sharp-edged dielectric wedge.

Solutions to Eq. (7) are Mathieu functions with imaginary order (a linear combination of two independent solutions):

$$g(\eta) = A\,\mathrm{ce}_{\mathrm{in}}(\eta,q) + B\,\mathrm{se}_{\mathrm{in}}(\eta,q) \tag{11}$$

with

$$\mathrm{ce}_{\mathrm{in}}(\eta,q) = \cosh(\nu_n\eta) + \sum_{r=1}^{\infty} q^r c_r(\eta) \ , \tag{12}$$

$$\mathrm{se}_{\mathrm{in}}(\eta,q) = \sinh(\nu_n\eta) + \sum_{r=1}^{\infty} q^r s_r(\eta) \ . \tag{13}$$

A and B are constants, and $-E_n = -\nu_n^2 + \sum_{r=1}^{\infty}\alpha_r q^r$, following the notation given by McLachlan.[11] The coefficients $c_r(\eta)$ and $s_r(\eta)$ are given in McLachlan's book,[11] with only the exchange of the imaginary index for a real one.

These solutions have well-defined properties of symmetry about the midplane of the dielectric (vacuum), defined by $\eta = 0$ ($\eta = \pi$). Equation (12) is associated with an even solution, and Eq. (13) corresponds to an odd solution, as in Dobrzynski and Maradudin's paper.[1] The series (12) and (13) converge if q is small, and diverge if q is large enough (note that close to the wedge q is always small).

Solutions to Eq. (8) can be obtained in a similar fashion. However, we are interested in an expression which contains the K Bessel functions as a limit for small values of h. We proceed as follows. With the change

$$u = 2\sqrt{-q}\,\cosh\xi = kh\cosh\xi \ , \tag{14}$$

Eq. (8) gives

$$u^2\frac{d^2f}{du^2} + u\frac{df}{du} - (u^2 - E_n + 2q) = -4q\frac{d^2f}{du^2} \ . \tag{15}$$

Equation (15) can be recognized as a modified Bessel equation with an inhomogeneous term.[12] In this case, we obtain the inhomogeneous solution f^{inh} if two linearly independent solutions of the homogeneous equation are known:[13]

$$f^{\mathrm{inh}}(u) = K_{i\alpha}(u)\int^u dt\, I_{i\alpha}(t)\left[\frac{4q}{t}\frac{d^2f^{\mathrm{inh}}(t)}{dt^2}\right] - I_{i\alpha}(u)\int^u dt\, K_{i\alpha}(t)\left[\frac{4q}{t}\frac{d^2f^{\mathrm{inh}}(t)}{dt^2}\right] + \mathrm{const} \ , \tag{16}$$

where

$$\alpha = (E_n + k^2h^2/2)^{1/2} \ . \tag{17}$$

From the asymptotic behavior of the I and K Bessel functions for large arguments[12] we select the $K_{i\alpha}$ function as the physical solution to the homogeneous part of Eq. (15), because $I_{i\alpha}$ grows exponentially for zones away from the edge of the hyperbolic dielectric wedge. Then, we can write the solution to the original differential equation (8) as

$$f(u)=\text{const}\times K_{i\alpha}(u)+f^{\text{inh}}(u) \quad . \tag{18}$$

To determine $f^{\text{inh}}(u)$, we must use Eq. (16), i.e., an integrodifferential equation. In order to study the behavior of the solution given in Eq. (16), we use a perturbative approach. The first-order approximation is obtained by substituting for f^{inh} in the right-hand side of Eq. (16) the solution of the homogeneous equation, $K_{i\alpha}(u)$. This leads to

$$f_1^{\text{inh}}(u)=qI_{i\alpha}(u)\int_u^\infty dt\,K_{i\alpha}(t)\frac{1}{t}[K_{i\alpha-2}(t)+2K_{i\alpha}(t)+K_{i\alpha+2}(t)] - qK_{i\alpha}(u)\int_u^\infty dt\,I_{i\alpha}(t)\frac{1}{t}[K_{i\alpha-2}(t)+2K_{i\alpha}(t)+K_{i\alpha+2}(t)] \quad , \tag{19}$$

where we have chosen the constant in Eq. (16) to avoid divergence problems as $u\rightarrow\infty$. This first-order approximation appears as a product of q times a nondivergent function of u, which implies that when $h\rightarrow 0$, then, from expression (9), $q\rightarrow 0$ and $f_1^{\text{inh}}\rightarrow 0$. Therefore, the solution to Eq. (8) in the limit $h\rightarrow 0$ is, according to Eq. (18),

$$f(r)\cong\text{const}\times K_{i\nu}(kr) \quad , \tag{20}$$

where ν is the continuous separation constant in Laplace's equation, as for the case $h\rightarrow 0$ (Ref. 1).

Now we return to the finite-h case. The even electrostatic potential has the form

$$\phi_n^e(\xi,\eta,z;t)=\begin{cases} Af(\xi)\text{ce}_{\text{in}}(\eta,q)\exp[i(kz-\omega t)] \;, & -\alpha<\eta<\alpha \;, \quad (21)\\ Bf(\xi)\text{ce}_{\text{in}}(\pi-\eta,q)\exp[i(kz-\omega t)] \;, & \alpha<\eta<2\pi-\alpha \;. \quad (22)\end{cases}$$

The odd electrostatic potential has the form

$$\phi_n^o(\xi,\eta,z;t)=\begin{cases} Cf(\xi)\text{se}_{\text{in}}(\eta,q)\exp[i(kz-\omega t)] \;, & -\alpha<\eta<\alpha \;, \quad (23)\\ Df(\xi)\text{se}_{\text{in}}(\pi-\eta,q)\exp[i(kz-\omega t)] \;, & \alpha<\eta<2\pi-\alpha \;, \quad (24)\end{cases}$$

with $f(\xi)$, $\text{ce}_{\text{in}}(\eta,q)$, and $\text{se}_{\text{in}}(\eta,q)$ given in expressions (18), (19), (12), and (13), respectively. By applying the boundary conditions we obtain the dispersion relation for the even and odd modes

$$\epsilon=-\frac{\text{ce}_{\text{in}}(\alpha,q)\text{ce}'_{\text{in}}(\pi-\alpha,q)}{\text{ce}'_{\text{in}}(\alpha,q)\text{ce}_{\text{in}}(\pi-\alpha,q)} \quad \text{(even modes)} \;, \tag{25}$$

$$\epsilon=-\frac{\text{se}_{\text{in}}(\alpha,q)\text{se}'_{\text{in}}(\pi-\alpha,q)}{\text{se}'_{\text{in}}(\alpha,q)\text{se}_{\text{in}}(\pi-\alpha,q)} \quad \text{(odd modes)} \;, \tag{26}$$

where ϵ is the dielectric function of the medium and the prime denotes derivation with respect to η. In the limit $h\rightarrow 0$, when the hyperbolic dielectric wedge tends to a sharp wedge, the dispersion relations (25) and (26) tend to the dispersion relations for the sharp wedge.[1]

The dispersion relation obtained by substituting the values of the ce_{in} and se_{in} functions (and the derivatives) calculated using Eqs. (10) to (13) with a few terms in the expansions, give a result in accordance with Davis's[2] dispersion relation for values of kh near unity. However, for kh away from this value, we need to use more terms in the series expansions in Eq. (10).

Therefore, the method proposed here to solve the electrostatic edge modes of the hyperbolic dielectric wedge gives *analytical* solutions, which reproduce correctly the analytical expressions obtained for the dielectric sharp wedge,[1]

The results obtained by this method can be used to study the interaction of an electron beam with a hyperbolic dielectric wedge, similarly to the analysis of Garcia-Molina, Gras-Marti, and Ritchie[7] of the interaction of an electron beam with a parabolic wedge. These studies are of great interest in scanning transmission electron microscopy experiments.[6,14]

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