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Vibrational Edge Modes in Finite Crystals

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In addition to surfaces, real crystals have edges, corners, and steps. In this paper we present a theory of long-wavelength acoustic phonons localized at an edge of a cubic elastic medium bounded by two (100) faces. The stress-free boundary conditions on the faces of the semi-infinite medium meeting at the edge are incorporated into the equations of motion of the medium by the device of assuming position-dependent elastic constants. The equations of motion of the medium are solved by expanding each displacement component in a double series of Laguerre functions, which are orthonormal and complete in the region $x_1 \geq 0$, $x_2 \geq 0$. The edge modes obtained are wavelike parallel to the edge and decay rapidly with increasing distance into the medium from the edge. For the particular case of an elastically isotropic medium for which the Lamé constants λ and μ are equal, the speed of propagation of the lowest-frequency edge mode is $0.9013c_t$, where c_t is the speed of sound of bulk transverse modes and is lower than that of Rayleigh waves, which is $0.9194c_t$. A variational principle for the speeds of edge modes is also presented.

I. INTRODUCTION

In recent years many investigations have been undertaken on the properties of excitations localized at crystal surfaces, such as surface phonons[1] and surface magnons.[2] If the surface is planar, these surface excitations have amplitudes which are wavelike parallel to the surface and which decay essentially exponentially in the normal direction away from the surface.

In addition to surfaces, however, real crystals may have edges, corners, and steps. The present paper is concerned with a theoretical study of phonons localized at an edge of a crystal. These edge excitations are characterized by a one-dimensional wave vector parallel to the edge and by rapidly decaying amplitudes in directions normal to the edge.

To simplify the analysis we assimilate the crystal into an elastic continuum and solve the equations of motion of a right-angle elastic wedge, together with stress-free boundary conditions on the faces which intersect at the edge. Our results, therefore, describe long-wavelength acoustic edge modes in a crystal.

II. VIBRATIONAL EDGE MODES

The equations of motion of an elastic continuum are

$$\rho \ddot{u}_\alpha = \sum_\beta \frac{\partial T_{\alpha\beta}}{\partial x_\beta} , \tag{2.1}$$

where $u_\alpha(\vec{x})$ is the α Cartesian component of the displacement field at the point $\vec{x}$, ρ is the mass density, and $T_{\alpha\beta}(\vec{x})$ is the stress tensor. The latter can be written in the form

$$T_{\alpha\beta}(\vec{x}) = \sum_{\mu\nu} C_{\alpha\beta\mu\nu}(\vec{x}) \eta_{\mu\nu}(\vec{x}) , \tag{2.2}$$

where the $\{C_{\alpha\beta\mu\nu}(\vec{x})\}$ are the elastic constants and $\eta_{\mu\nu}(\vec{x})$ is an element of the strain tensor

$$\eta_{\mu\nu} = \frac{1}{2}\left(\frac{\partial u_\mu}{\partial x_\nu} + \frac{\partial u_\nu}{\partial x_\mu} \right) . \tag{2.3}$$

When Eqs. (2.2) and (2.3) are substituted into Eq. (2.1) we obtain the equations

$$\rho \ddot{u} = \sum_{\beta\mu\nu} \frac{\partial C_{\alpha\beta\mu\nu}}{\partial x_\beta} \frac{\partial u_\mu}{\partial x_\nu} + \sum_{\beta\mu\nu} C_{\alpha\beta\mu\nu} \frac{\partial^2 u_\mu}{\partial x_\beta \partial x_\nu} . \tag{2.4}$$

If we consider a semi-infinite solid occupying the quadrant $x_1 \geq 0$, $x_2 \geq 0$, $-\infty < x_3 < \infty$, the position dependence of the elastic constants is given by

$$C_{\alpha\beta\mu\nu}(\vec{x}) = \Theta(x_1)\,\Theta(x_2) C_{\alpha\beta\mu\nu} , \tag{2.5}$$

where $\Theta(x)$ is the Heaviside unit step function and the $\{C_{\alpha\beta\mu\nu}\}$ are the ordinary (position-independent) elastic constants of the medium. Combining Eqs. (2.4) and (2.5) we obtain as the equations of motion of an elastic continuum occupying the region $x_1,\ x_2 \geq 0$, with an edge along the x_3 axis,

$$\rho \ddot{u}_\alpha = \delta(x_1) \sum_{\mu\nu} C_{\alpha 1\mu\nu} \frac{\partial u_\mu}{\partial x_\nu} + \delta(x_2) \sum_{\mu\nu} C_{\alpha 2\mu\nu} \frac{\partial u_\mu}{\partial x_\nu} + \sum_{\beta\mu\nu} C_{\alpha\beta\mu\nu} \frac{\partial^2 u_\mu}{\partial x_\beta \partial x_\nu} , \quad x_1, x_2 \geq 0 . \tag{2.6}$$

Solving Eq. (2.6) with the first two terms on the right-hand side present is equivalent to solving the usual equations of motion for an elastic medium and then imposing the conditions that the surfaces $x_1 = 0$ ($x_2 \geq 0$) and $x_2 = 0$ ($x_1 \geq 0$) be stress free. This is because the coefficients of $\delta(x_1)$ and $\delta(x_2)$ are the components of the stresses acting on these two surfaces, respectively. The formal device of introducing position-dependent elastic constants has been used previously in other studies of the vibrations of semi-infinite elastic media.[3] It is convenient to use it in the present work because by incorporating the boundary conditions in the equations of motion it makes possible the semi-variational determination of the frequencies of edge modes, to a discussion of which we now turn.

In what follows, rather than maintaining complete generality we specialize to the case of a cubic medium for which the cube axes and the coordinate axes coincide.

We assume as a solution to Eqs. (2.6)

$$u_\alpha(\vec{x}, t) = \bar{u}_\alpha(x_1, x_2)\exp(iqx_3 - i\omega t) , \tag{2.7}$$

and find that the equations satisfied by the amplitude functions $\{\bar{u}_\alpha(x_1, x_2)\}$ are

$$-\rho\omega^2\bar{u}_1 = \delta(x_1)\left(c_{11}\frac{\partial\bar{u}_1}{\partial x_1} + c_{12}\frac{\partial\bar{u}_2}{\partial x_2} + iqc_{12}\bar{u}_3\right) + \delta(x_2)c_{44}\left(\frac{\partial\bar{u}_1}{\partial x_2} + \frac{\partial\bar{u}_2}{\partial x_1}\right)$$
$$+\left(c_{11}\frac{\partial^2\bar{u}_1}{\partial x_1^2} + c_{44}\frac{\partial^2\bar{u}_1}{\partial x_2^2} - q^2c_{44}\bar{u}_1 + (c_{12}+c_{44})\frac{\partial^2\bar{u}_2}{\partial x_1\partial x_2} + iq(c_{12}+c_{44})\frac{\partial\bar{u}_3}{\partial x_1}\right) , \tag{2.8a}$$

$$-\rho\omega^2\bar{u}_2 = \delta(x_1)c_{44}\left(\frac{\partial\bar{u}_1}{\partial x_2} + \frac{\partial\bar{u}_2}{\partial x_1}\right) + \delta(x_2)\left(c_{12}\frac{\partial\bar{u}_1}{\partial x_1} + c_{11}\frac{\partial\bar{u}_2}{\partial x_2} + iqc_{12}\bar{u}_3\right)$$
$$+\left((c_{12}+c_{44})\frac{\partial^2\bar{u}_1}{\partial x_1\partial x_2} + c_{44}\frac{\partial^2\bar{u}_2}{\partial x_1^2} + c_{11}\frac{\partial^2\bar{u}_2}{\partial x_2^2} - q^2c_{44}\bar{u}_2 + iq(c_{12}+c_{44})\frac{\partial\bar{u}_3}{\partial x_2}\right) , \tag{2.8b}$$

$$-\rho\omega^2\bar{u}_3 = \delta(x_1)c_{44}\left(iq\bar{u}_1 + \frac{\partial\bar{u}_3}{\partial x_1}\right) + \delta(x_2)c_{44}\left(iq\bar{u}_2 + \frac{\partial\bar{u}_3}{\partial x_2}\right)$$
$$+\left(iq(c_{12}+c_{44})\frac{\partial\bar{u}_1}{\partial x_1} + iq(c_{12}+c_{44})\frac{\partial\bar{u}_2}{\partial x_2} + c_{44}\frac{\partial^2\bar{u}_3}{\partial x_1^2} + c_{44}\frac{\partial^2\bar{u}_3}{\partial x_2^2} - q^2c_{11}\bar{u}_3\right) , \tag{2.8c}$$

where the c_{ij} are the elastic constants in the contracted (Voigt) notation.

We now introduce the changes of variables

$$x_1 = \xi/q, \quad x_2 = \eta/q , \tag{2.9}$$

and define new coefficient functions $\{\hat{u}_\alpha(\xi, \eta)\}$ by

$$\bar{u}_1(x_1, x_2) = \hat{u}_1(\xi, \eta), \quad \bar{u}_2(x_1, x_2) = \hat{u}_2(\xi, \eta) ,$$
$$i\bar{u}_3(x_1, x_2) = \hat{u}_3(\xi, \eta) , \tag{2.10}$$

to obtain

$$-\rho\frac{\omega^2}{q^2}\hat{u}_1 = \delta(\xi)\left(c_{11}\frac{\partial\hat{u}_1}{\partial\xi} + c_{12}\frac{\partial\hat{u}_2}{\partial\eta} + c_{12}\hat{u}_3\right) + \delta(\eta)c_{44}\left(\frac{\partial\hat{u}_1}{\partial\eta} + \frac{\partial\hat{u}_2}{\partial\xi}\right)$$
$$+\left(c_{11}\frac{\partial^2\hat{u}_1}{\partial\xi^2} + c_{44}\frac{\partial^2\hat{u}_1}{\partial\eta^2} - c_{44}\hat{u}_1 + (c_{12}+c_{44})\frac{\partial^2\hat{u}_2}{\partial\xi\,\partial\eta} + (c_{12}+c_{44})\frac{\partial\hat{u}_3}{\partial\xi}\right), \tag{2.11a}$$

$$-\rho\frac{\omega^2}{q^2}\hat{u}_2 = \delta(\xi)c_{44}\left(\frac{\partial\hat{u}_1}{\partial\eta} + \frac{\partial\hat{u}_2}{\partial\xi}\right) + \delta(\eta)\left(c_{12}\frac{\partial\hat{u}_1}{\partial\xi} + c_{11}\frac{\partial\hat{u}_2}{\partial\eta} + c_{12}\hat{u}_3\right)$$
$$+\left(c_{12}+c_{44})\frac{\partial^2\hat{u}_1}{\partial\xi\,\partial\eta} + c_{11}\frac{\partial^2\hat{u}_2}{\partial\eta^2} + c_{44}\frac{\partial^2\hat{u}_2}{\partial\xi^2} - c_{44}\hat{u}_2 + (c_{12}+c_{44})\frac{\partial\hat{u}_3}{\partial\eta}\right) , \tag{2.11b}$$

$$-\rho\frac{\omega^2}{q^2}\hat{u}_3 = \delta(\xi)c_{44}\left(-\hat{u}_1 + \frac{\partial\hat{u}_3}{\partial\xi}\right) + \delta(\eta)c_{44}\left(-\hat{u}_2 + \frac{\partial\hat{u}_3}{\partial\eta}\right)$$
$$+\left(-(c_{12}+c_{44})\frac{\partial\hat{u}_1}{\partial\xi} - (c_{12}+c_{44})\frac{\partial\hat{u}_2}{\partial\eta} + c_{44}\frac{\partial^2\hat{u}_3}{\partial\xi^2} + c_{44}\frac{\partial^2\hat{u}_3}{\partial\eta^2} - c_{11}\hat{u}_3\right) . \tag{2.11c}$$

From these equations we see that ω is linear in q.

To solve this system of equations we expand $\hat{u}_\alpha(\xi, \eta)$ as

$$\hat{u}_\alpha(\xi, \eta) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} a_{mn}^{(\alpha)}\phi_m(\xi)\,\phi_n(\eta) , \tag{2.12}$$

where

$$\phi_m(\xi) = e^{-\xi/2}\,[L_m(\xi)/m!] = |m\rangle \tag{2.13}$$

and $L_m(\xi)$ is the mth Laguerre polynomial. The choice of the expansion (2.12) was dictated by the fact that the set of functions $\{\phi_m(\xi)\}$ is orthonormal and complete in the interval $0 \leq \xi \leq \infty$, and so is well suited for the expansion of a function defined only for positive values of ξ and η. In addition, the presence of the factor $e^{-\xi/2}$ in the definition of $\phi_m(\xi)$ is convenient since we are looking for functions localized in the vicinity of the edge.

The generating function for the $\{\phi_m(\xi)\}$ is

$$\frac{\exp[-\frac{1}{2}\xi(1+s)/(1-s)]}{1-s} = \sum_{m=0}^{\infty} s^m \phi_m(\xi) . \quad (2.14)$$

The first few of these functions are

$$\begin{aligned} \phi_0(\xi) &= e^{-\xi/2} , \\ \phi_1(\xi) &= e^{-\xi/2}(1-\xi) , \\ \phi_2(\xi) &= e^{-\xi/2}(1-2\xi+\tfrac{1}{2}\xi^2) , \\ \phi_3(\xi) &= e^{-\xi/2}(1-3\xi+\tfrac{3}{2}\xi^2-\tfrac{1}{6}\xi^3) \cdots . \end{aligned} \quad (2.15)$$

The recurrence formula satisfied by the $\{\phi_m(\xi)\}$ is

$$\phi_{m+1}(\xi) = \frac{2m+1-\xi}{m+1}\,\phi_m(\xi) - \frac{m}{m+1}\,\phi_{m-1}(\xi) . \quad (2.16)$$

With the aid of the generating function (2.14) the following useful matrix elements are readily obtained:

$$\begin{aligned} \langle m | n\rangle &= \delta_{mn} , \\ \langle m | \delta(\xi) | n\rangle &= 1 , \\ \left\langle m \middle| \delta(\xi)\frac{d}{d\xi} \middle| n\right\rangle &= -(n+\tfrac{1}{2}) , \\ \left\langle m \middle| \frac{d}{d\xi} \middle| n\right\rangle &= -[\tfrac{1}{2}\delta_{mn}+\Theta(n-m-1)] , \\ \left\langle m \middle| \frac{d^2}{d\xi^2} \middle| n\right\rangle &= \tfrac{1}{4}\delta_{mn}+(n-m)\,\Theta(n-m-1) , \end{aligned} \quad (2.17)$$

where

$$\begin{aligned} \Theta(n) &= 1, \quad n \geq 0 \\ &= 0, \quad n < 0 . \end{aligned}$$

When the expansion (2.12) is substituted into Eqs. (2.11) and the orthonormality of the $\{\phi_m(\xi)\}$ is used, the resulting equations for the expansion coefficients can be written in the form

$$\Omega^2 a_{ij}^{(\alpha)} = \sum_{\beta=1}^{3}\sum_{m,n} A_{ij;mn}^{(\alpha\beta)} a_{mn}^{(\beta)}, \quad \alpha = 1, 2, 3 \quad (2.18)$$

where

$$\Omega^2 = \rho\omega^2/c_{44}q^2 . \quad (2.19)$$

The matrix elements $\{A_{ij;mn}^{(\alpha\beta)}\}$ are given by

$$\begin{aligned} A_{ij;mn}^{(11)} &= \tfrac{1}{4}(3-A)\,\delta_{im}\delta_{jn} + A\delta_{jn}[\min(i,m)+\tfrac{1}{2}] \\ &\quad + \delta_{im}[\min(j,n)+\tfrac{1}{2}] , \\ A_{ij;mn}^{(12)} &= [\tfrac{1}{2}\delta_{im}+\Theta(m-i-1)] + B[\tfrac{1}{2}\delta_{jn}+\Theta(n-j-1)] \\ &\quad - (B+1)[\tfrac{1}{2}\delta_{im}+\Theta(m-i-1)][\tfrac{1}{2}\delta_{jn}+\Theta(n-j-1)] , \\ A_{ij;mn}^{(13)} &= \delta_{im}\delta_{jn}\tfrac{1}{2}(B+1) + \delta_{jn}[-B+(B+1)\,\Theta(m-i-1)] , \\ A_{ij;mn}^{(21)} &= A_{ji;nm}^{(12)} , \\ A_{ij;mn}^{(22)} &= A_{ji;nm}^{(11)} , \\ A_{ij;mn}^{(23)} &= A_{ji;nm}^{(13)} , \\ A_{ij;mn}^{(31)} &= -\delta_{im}\delta_{jn}\tfrac{1}{2}(B+1) + \delta_{jn}[1-(B+1)\,\Theta(m-i-1)] , \\ A_{ij;mn}^{(32)} &= A_{ji;nm}^{(31)} , \\ A_{ij;mn}^{(33)} &= (A-\tfrac{1}{2})\,\delta_{im}\delta_{jn} + \delta_{im}[\min(j,n)+\tfrac{1}{2}] \\ &\quad + \delta_{jn}[\min(i,m)+\tfrac{1}{2}] , \end{aligned} \quad (2.20)$$

where we have set

$$A = c_{11}/c_{44}, \quad B = c_{12}/c_{44} . \quad (2.21)$$

It should be noted that for arbitrary values of A and B the matrix $A_{ij;mn}^{(\alpha\beta)}$ is not symmetric, that is to say we have

$$A_{ij;mn}^{(\alpha\beta)} \neq A_{mn;ij}^{(\beta\alpha)} .$$

However, in the special case $A=3$, $B=1$, to be discussed below, this matrix is symmetric: $A_{ij;mn}^{(\alpha\beta)} = A_{mn;ij}^{(\beta\alpha)}$.

Equations (2.18)–(2.21) can be simplified somewhat by the use of symmetry and group theory. The wedge $x_1 \geq 0$, $x_2 \geq 0$, $-\infty < x_3 < \infty$, is invariant under the operations of the point group C_s, whose elements are E, the identity, and σ, the reflection in the plane containing the x_3 axis and bisecting the x_1 and x_2 axes. If we write Eqs. (2.11) in the form

$$-\rho\omega^2 \hat{u}_\alpha(\xi,\eta) = \textstyle\sum_\beta L_{\alpha\beta}(\xi,\eta)\,\hat{u}_\beta(\xi,\eta) , \quad (2.22)$$

which defines the differential operators $\{L_{\alpha\beta}(\xi,\eta)\}$ implicitly, it can be shown straightforwardly that these operators transform under the operations of the group C_s according to

$$L_{\alpha\beta}(S\vec{x}_\parallel) = \sum_{\mu\nu} S_{\alpha\mu} S_{\beta\nu} L_{\mu\nu}(\vec{x}_\parallel) , \quad (2.23)$$

where S is the 3×3 real orthogonal matrix representative of an operation of the group C_s and $\vec{x}_\parallel$ is the vector $(\xi,\eta,0)$. Combining Eqs. (2.22) and (2.23) we obtain

$$-\rho\omega^2 \textstyle\sum_\alpha S_{\mu\alpha}^{-1}\,\hat{u}_\alpha(S\vec{x}_\parallel) = \sum_\nu L_{\mu\nu}(\vec{x}_\parallel) \sum_\beta S_{\nu\beta}^{-1}\,\hat{u}_\beta(S\vec{x}_\parallel) . \quad (2.24)$$

Thus, if $\hat{\vec{u}}(\vec{x}_\parallel)$ is a solution of Eq. (2.22) with frequency ω, so is $S^{-1}\hat{\vec{u}}(S\vec{x}_\parallel)$. Consequently, the components of $\hat{\vec{u}}(\vec{x}_\parallel)$ are basis functions for the irreducible representations of C_s. The group C_s has only two one-dimensional irreducible representations, Γ_1 and Γ_2,[4] and we are led to the results that the displacement fields belonging to these two representations possess the properties

$$\begin{aligned} \Gamma_1:\quad & \hat{u}_1(\eta,\xi) = \hat{u}_2(\xi,\eta) , \\ & \hat{u}_2(\eta,\xi) = \hat{u}_1(\xi,\eta) , \\ & \hat{u}_3(\eta,\xi) = \hat{u}_3(\xi,\eta) ; \end{aligned}$$

$$\Gamma_2:\ \hat{u}_1(\eta,\xi) = -\hat{u}_2(\xi,\eta)\ ,$$
$$\hat{u}_2(\eta,\xi) = -\hat{u}_1(\xi,\eta)\ ,$$
$$\hat{u}_3(\eta,\xi) = -\hat{u}_3(\xi,\eta)\ . \qquad (2.25)$$

These conditions translate into the following conditions on the coefficients $\{a^{(\alpha)}_{mn}\}$ in the expansions (2.12):

$$a^{(1)}_{nm} = \pm a^{(2)}_{mn}\ ,$$
$$a^{(2)}_{nm} = \pm a^{(1)}_{mn}\ , \qquad (2.26)$$
$$a^{(3)}_{nm} = \pm a^{(3)}_{mn}\ ,$$

where the upper (lower) signs refer to displacements belonging to $\Gamma_1(\Gamma_2)$. The use of Eqs. (2.26) together with Eqs. (2.18)–(2.21) allows one to work with matrices of about half the dimensionality required when no account is taken of Eqs. (2.26).

In the present work Eqs. (2.26) were used to simplify Eqs. (2.18)–(2.21), but not to the fullest extent possible. The equations that were solved are

$$\Omega^2 a^{(1)}_{ij} = \sum_{mn} \{B^{(11)}_{ij;mn} a^{(1)}_{mn} + B^{(13)}_{ij;mn} a^{(3)}_{mn}\}\ ,$$
$$\Omega^2 a^{(3)}_{ij} = \sum_{mn} \{B^{(31)}_{ij;mn} a^{(1)}_{mn} + B^{(33)}_{ij;mn} a^{(3)}_{mn}\}\ , \qquad (2.27)$$

and $a^{(2)}_{ij}$ was obtained from $a^{(1)}_{ij}$ by means of Eqs. (2.26). The matrix elements $\{B^{(\alpha\beta)}_{ij;mn}\}$ appearing in these equations are given by

$$B^{(11)}_{ij;mn} = A^{(11)}_{ij;mn} + A^{(12)}_{ij;nm}\ ,$$
$$B^{(13)}_{ij;mn} = \tfrac{1}{2}(A^{(13)}_{ij;mn} + A^{(13)}_{ij;nm})\ , \qquad (2.28)$$
$$B^{(31)}_{ij;mn} = \tfrac{1}{2}(A^{(31)}_{ij;mn} + A^{(32)}_{ij;nm} + A^{(31)}_{ji;mn} + A^{(32)}_{ji;nm}\ ,$$
$$B^{(33)}_{ij;mn} = \tfrac{1}{4}(A^{(33)}_{ij;mn} + A^{(33)}_{ij;nm} + A^{(33)}_{ji;mn} + A^{(33)}_{ji;nm})\ ,$$

for modes of Γ_1 symmetry, and by

$$B^{(11)}_{ij;mn} = A^{(11)}_{ij;mn} - A^{(12)}_{ij;nm}\ ,$$
$$B^{(13)}_{ij;mn} = \tfrac{1}{2}(A^{(13)}_{ij;mn} - A^{(13)}_{ij;nm})\ , \qquad (2.29)$$
$$B^{(31)}_{ij;mn} = \tfrac{1}{2}(A^{(31)}_{ij;mn} - A^{(32)}_{ij;nm} - A^{(31)}_{ji;mn} + A^{(32)}_{ji;nm})\ ,$$
$$B^{(33)}_{ij;mn} = \tfrac{1}{4}(A^{(33)}_{ij;mn} - A^{(33)}_{ij;nm} - A^{(33)}_{ji;mn} + A^{(33)}_{ji;nm})\ ,$$

for modes of Γ_2 symmetry. The use of Eqs. (2.27)–(2.29) in place of Eqs. (2.18) results in a reduction in the dimensionality of the matrices to be diagonalized by a factor of one-third, for the same number of terms in the expansions (2.12).

We have solved the set of equations (2.27)–(2.29) to obtain the lowest few eigenvalues and the corresponding eigenvectors for the special case $A=3$, $B=1$. This is the so-called Poisson case in which the elastic constants satisfy the isotropy condition and the Cauchy relations. (The Lamé constants λ and μ characterizing the elastic properties of an isotropic medium are equal in this case.) The expansion (2.12) was truncated by retaining all terms for which $m+n \le p$ ($m \ge 0$, $n \ge 0$, $p \ge 0$). Consequently, for a given value of p there are $\frac{1}{2}(p+1) \times (p+2)$ terms in the expansion (2.12) for each component $\hat{u}_\alpha(\xi,\eta)$, and the dimensionality of the corresponding matrix equation (2.27) is therefore $(p+1)(p+2) \times (p+1)(p+2)$.

The results of the calculations show that the lowest-frequency edge mode has Γ_2 symmetry; the edge mode of next lowest frequency has Γ_1 symmetry. To show how rapidly the calculations converge with increasing p we present in Table I the values of the two lowest eigenvalues as functions of p. (Note that the calculations for $p=11$ required the diagonalization of a 156×156 matrix.)

Because for the choice of A and B made here the speed of sound for bulk transverse waves is

$$c_t = (c_{44}/\rho)^{1/2}\ , \qquad (2.30)$$

we see from Eq. (2.19) that the dispersion relation for edge modes is given by

$$\omega = \Omega c_t q\ , \qquad (2.31)$$

where Ω^2 is an eigenvalue of the matrix $A^{(\alpha\beta)}_{ij;mn}$.

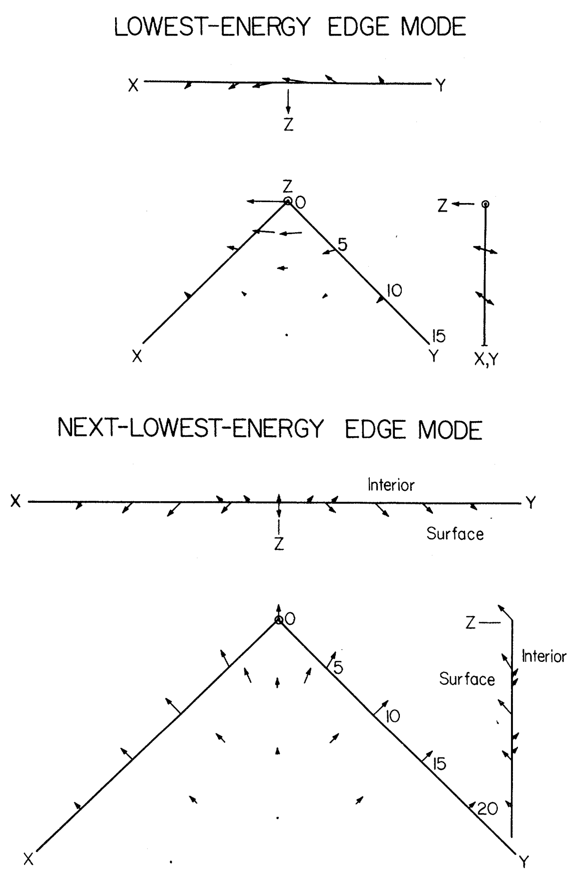

FIG. 1. Displacement fields of (a) the vibrational edge mode of lowest frequency possessing Γ_2 symmetry, and (b) the vibrational edge mode of lowest frequency possessing Γ_1 symmetry.

TABLE I. The values of the lowest (Γ_2) and next-lowest (Γ_1) eigenvalues of the matrix $\underline{A}$ defined by Eqs. (2.18)–(2.21) as functions of the number of terms retained in the expansions (2.12) of the displacement amplitudes.

p	$\Omega^2(\Gamma_2)$	$\Omega^2(\Gamma_1)$
0		
1	0.8788	1.1061
2	0.8227	0.9130
3	0.8140	0.8854
4	0.8131	0.8675
5	0.8128	0.8612
6	0.8127	0.8566
7	0.8126	0.8540
8	0.8124	0.8520
9	0.8124	0.8507
10	0.8124	0.8496
11	0.8124	0.8491

From the results of Table I we find that the frequencies of the two lowest edge modes are

$$\omega_{E_1} = 0.9013 c_t q \ , \qquad \omega_{E_2} = 0.9215 c_t q \ . \tag{2.32}$$

These results should be compared with the frequency of Rayleigh waves of the same wave vector[5]:

$$\omega_R = 0.9194 c_t q \ . \tag{2.33}$$

Thus we see that the speed of the lowest-frequency edge mode is slower than that of Rayleigh waves, while that of the next-highest-frequency edge mode is slightly faster.

It is found numerically that the frequencies of the modes of Γ_1 symmetry interlace those of the modes of Γ_2 symmetry, at least for the ten or so lowest-frequency edge modes. We have not been able to determine whether this result holds for all edge modes or not.

The displacement patterns corresponding to the two lowest-frequency edge modes are plotted in Fig. 1 (calculated from the results for $p=8$), and the rapid decay of the displacement amplitudes with increasing distance from the edge is clearly evident from these plots.

III. VARIATIONAL APPROACH TO VIBRATIONAL EDGE MODES

It is possible to formulate the problem of obtaining vibrational edge modes variationally. For this we first consider the functional

$$F(\vec{u}(\vec{x})) = \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \times \sum_{\alpha\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \left(\frac{\partial u_\alpha}{\partial x_\beta}\right)^* \left(\frac{\partial u_\gamma}{\partial u_\delta}\right) \ , \tag{3.1}$$

where L is the periodicity length of the elastic medium parallel to the edge. We now let $u_\alpha(\vec{x})$ go into $u_\alpha(\vec{x}) + \delta u_\alpha(\vec{x})$, whereupon $F(\vec{u}(\vec{x}))$ goes into $F(\vec{u}(\vec{x})) + \delta F(\vec{u}(\vec{x}))$, where

$$\delta F(\vec{u}(\vec{x})) = \sum_{\alpha\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \left(\frac{\partial u_\alpha^*}{\partial x_\beta} \frac{\partial}{\partial x_\delta} \delta u_\gamma + \frac{\partial u_\gamma}{\partial x_\delta} \frac{\partial}{\partial x_\beta} \delta u_\alpha^* \right) \ . \tag{3.2}$$

We integrate by parts to obtain

$$\begin{aligned}
\delta F(\vec{u}(\vec{x})) = &- \sum_{\alpha\gamma\delta} \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \, \delta u_\alpha^* C_{\alpha 1 \gamma\delta} \frac{\partial u_\gamma}{\partial x_\delta}\bigg|_{x_1=0} - \sum_{\alpha\gamma\delta} \int_0^\infty dx_1 \int_{-L/2}^{L/2} dx_3 \, \delta u_\alpha^* C_{\alpha 2\gamma\delta} \frac{\partial u_\gamma}{\partial x_\delta}\bigg|_{x_2=0} \\
&- \sum_{\alpha\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \, \delta u_\alpha^* C_{\alpha\beta\gamma\delta} \frac{\partial^2 u_\gamma}{\partial x_\beta \partial x_\delta} + \text{c.c.} \\
= &- \sum_{\alpha\gamma\delta} \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \, \delta u_\alpha^* \left(C_{\alpha 1\gamma\delta} \delta(x_1) \frac{\partial u_\gamma}{\partial x_\delta} + C_{\alpha 2\gamma\delta} \delta(x_2) \frac{\partial u_\gamma}{\partial x_\delta} \right) \\
&- \sum_{\alpha\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 \, \delta u_\alpha^* \frac{\partial^2 u_\gamma}{\partial x_\beta \partial x_\delta} + \text{c.c.}
\end{aligned} \tag{3.3}$$

The displacements $u_\alpha(\vec{x})$ and $u_\alpha^*(\vec{x})$ are linearly independent. Thus, if we minimize $F(\vec{u}(\vec{x}))$ with respect to variations of $\vec{u}^*(\vec{x})$, subject to the constraint

$$G(\vec{u}(\vec{x})) = \sum_\alpha \int_0^\infty dx_1 \int_0^\infty dx_2 \int_{-L/2}^{L/2} dx_3 u_\alpha^* u_\alpha = \text{const} \ , \tag{3.4}$$

the resulting Euler equation for determining $\vec{u}(\vec{x})$ becomes

$$-\sum_{\gamma\delta}\delta(x_1)C_{\alpha 1\gamma\delta}\frac{\partial u_\gamma}{\partial x_\delta}-\sum_{\gamma\delta}\delta(x_2)C_{\alpha 2\gamma\delta}\frac{\partial u_\gamma}{\partial x_\delta}-\sum_{\beta\gamma\delta}C_{\alpha\beta\gamma\delta}\frac{\partial^2 u_\gamma}{\partial x_\beta\,\partial x_\delta}-\lambda u_\alpha=0, \quad x_1, x_2\geq 0 \tag{3.5}$$

where λ is a Lagrange multiplier, which we can identify as $\rho\omega^2$.

Let us now consider the functional

$$\rho\Omega^2(\vec{u}(\vec{x}))=F(\vec{u}(\vec{x}))/G(\vec{u}(\vec{x})) \;. \tag{3.6}$$

Since $G(\vec{u}(\vec{x}))=\text{const}$ is just the normalization condition for $\vec{u}(\vec{x})$, the above variational procedure is equivalent to minimizing $\rho\Omega^2(\vec{u}(\vec{x}))$.

In fact, if we multiply the equation

$$\rho\omega^2 u_\alpha=-\delta(x_1)\sum_{\gamma\delta}C_{\alpha 1\gamma\delta}\frac{\partial u_\gamma}{\partial x_\delta}-\delta(x_2)\sum_{\gamma\delta}C_{\alpha 2\gamma\delta}\frac{\partial u_\gamma}{\partial x_\delta}-\sum_{\beta\gamma\delta}C_{\alpha\beta\gamma\delta}\frac{\partial^2 u_\gamma}{\partial x_\beta\,\partial x_\delta}, \quad x_1, x_2\geq 0 \tag{3.7}$$

[which is just Eq. (2.6) when a harmonic time dependence is assumed for $\vec{u}(\vec{x})$], by u_α^*, sum on α, and integrate over the region $0\leq x_1\leq\infty$, $0\leq x_2\leq\infty$, $-\frac{1}{2}L\leq x_3\leq\frac{1}{2}L$, we find after an integration by parts that the minimum value of $\Omega^2(\vec{u}(\vec{x}))$ is ω^2.

The symmetry properties of the displacement amplitudes expressed by Eqs. (2.25) should be taken into account in constructing the trial functions used in minimizing the functional $\rho\Omega^2(\vec{u}(\vec{x}))$.

IV. DISCUSSION

In this paper a method has been developed for obtaining the frequencies and the corresponding displacement fields for vibration modes localized at an edge formed by the intersection of two stress-free (100) surfaces of a cubic elastic medium. It has been applied to obtain the lowest edge-mode frequencies for an isotropic medium whose elastic constants satisfy the Poisson condition. It is found that the speed of sound for the lowest-frequency edge mode is lower than that of Rayleigh surface modes on the same wavelength.

Several interesting properties of edge modes remain to be studied. The dependence of the speed of the lowest-frequency edge modes on the elastic constants, even for cubic crystals, should be determined. The degree to which edge modes are localized in the vicinity of the edge undoubtedly depends on the elastic constants of the medium and on the angle of the wedge. We have considered only a right-angle wedge in this paper, and the question of whether edge modes are more localized, or less, when the wedge angle is acute or obtuse remains unanswered. For dealing with wedges other than right-angle wedges a transformation of the equations of motion to cylindrical coordinates would seem to be appropriate. It is hoped to consider these and other problems in a subsequent paper.

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[1]See, for example, A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, *Theory of Lattice Dynamics in the Harmonic Approximtion*, 2nd ed. (Academic, New York, 1971), Chap. IX.

[2]See, for example, R. F. Wallis, A. A. Maradudin, I. P. Ipatova, and A. A. Klochikhin, Solid State Commun. 5, 89 (1967).

[3]W. Ludwig and B. Lengeler, Solid State Commun. 2, 83 (1964); see also the discussion in A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, in Ref. 1, pp. 523–527.

[4]G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-two Point Groups* (MIT Press, Cambridge, Mass., 1963).

[5]A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (Dover, New York, 1944), p. 308.