Vibrational Edge Modes for Small-Angle Wedges

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Moss, Maradudin, and Cunningham recently calculated the velocities of long-wavelength acoustic phonons localized at the apex of a variable-angle semi-infinite elastic wedge. We present here a method by which more precise results may be obtained for small wedge angles.

Recently, Moss, Maradudin, and Cunningham[1] (hereafter referred to as I) performed numerical calculations to obtain the speeds of long-wavelength acoustic-phonon modes localized at the apex of a variable-angle semi-infinite wedge consisting of an isotropic cubic elastic medium. After mapping the wedge into a right-angle wedge, they solved the equations of motion by expanding the displacement components in a double series of Laguerre functions, $\varphi_k(x)=e^{-x/2}L_k(x)/k!$, where $L_k(x)$ is the kth Laguerre polynomial. For wedge angles of from 30° to 180° the convergence of the lowest eigenvalues given by this series was good. However, for angles of less than 30° the convergence was not very rapid, and the eigenvalues were estimated by visual extrapolation of the curves of eigenvalue versus p, where p is a measure of the number of terms taken in the double Laguerre expansions. The slow convergence of the expansions for small wedge angles is due to the fact that as the interior angle of the wedge decreases, the edge modes become more localized at the apex of the wedge, i.e., the displacement amplitudes decay more rapidly with distance into the wedge from its apex and from the plane faces that bound it. However, the exponential factor which multiplies the Laguerre polynomials in the Laguerre functions used to expand the displacement amplitudes has a fixed decay length, independent of wedge angle, for a given value of q, the wave-vector component parallel to the edge of the wedge. Consequently, to reproduce the more rapid decay of the displacement components with decreasing wedge angle, more Laguerre polynomials had to be retained in their expansions.

This suggests that an improvement in the rate of convergence of the series expansions for the displacement components could be achieved by decreasing the decay length in the exponential factor in the Laguerre functions with decreasing wedge angle, so that fewer terms in the expansions would be required. To achieve this, the change of variables,

$$\xi=\alpha\bar{\xi}\ , \tag{1a}$$

$$\eta=\alpha\bar{\eta}\ , \tag{1b}$$

was made in Eq. (I17). This variable change has the effect of introducing α into Eq. (I22) for the Laguerre function,

$$\varphi_k(x/\alpha)=\frac{e^{-x/2\alpha}L_k(x/\alpha)}{k!}\ . \tag{2}$$

Thus, by changing α it is possible to affect the rate of decay of the Laguerre functions, thereby improving the rate of convergence of the series. Following exactly the methods of I, we obtain the eigenvalue equation [Eq. (I23) is effectively Eq. (23) of I]

$$\Omega^2 a_{ij}^{(\alpha)}=\sum_{\beta=1}^{3}\sum_{k,l=0}^{\infty}A_{ij;kl}^{(\alpha\beta)}(m)a_{kl}^{(\beta)}\ ,\quad \alpha=1,2,3 \tag{I23}$$

for the expansion coefficients $\{a_{kl}^{(\alpha)}\}$ of the displacement amplitudes, where Ω^2 is given by

$$\Omega^2=\rho\omega^2/C_{44}q^2\ . \tag{I24}$$

From Eq. (I24) we see that Ω is the speed of propagation of the edge mode in units of the speed of the bulk transverse-acoustic mode in the [100] direction. In our calculations the sum on k and l in Eq. (I23) was restricted by the condition $0\leq k+l\leq p$.

With the change of variables of Eqs. (1), the matrix elements $\{A_{ij;kl}^{(\alpha\beta)}(m)\}$ are given by

$$A_{ij;kl}^{(11)}(m)=\frac{1}{\alpha^2}\{\text{Eq. (I25a)}\}+(1-1/\alpha^2)\delta_{ik}\delta_{jl}\ , \tag{3a}$$

$$A_{ij;kl}^{(12)}(m)=\frac{1}{\alpha^2}\{\text{Eq. (I25b)}\}\ , \tag{3b}$$

$$A_{ij;kl}^{(13)}(m)=\frac{1}{\alpha}\{\text{Eq. (I25c)}\}\ , \tag{3c}$$

$$A_{ij;kl}^{(21)}(m)=\frac{1}{\alpha^2}\{\text{Eq. (I25d)}\}\ , \tag{3d}$$

$$A_{ij;kl}^{(22)}(m)=A_{ji;lk}^{(11)}(m)\ , \tag{3e}$$

$$A_{ij;kl}^{(23)}(m)=\frac{1}{\alpha}\{\text{Eq. (I25f)}\}\ , \tag{3f}$$

$$A_{ij;kl}^{(31)}(m)=\frac{1}{\alpha}\{\text{Eq. (I25g)}\}\ , \tag{3g}$$

$$A_{ij;kl}^{(32)}(m)=A_{ji;kl}^{(31)}(m)\ , \tag{3h}$$

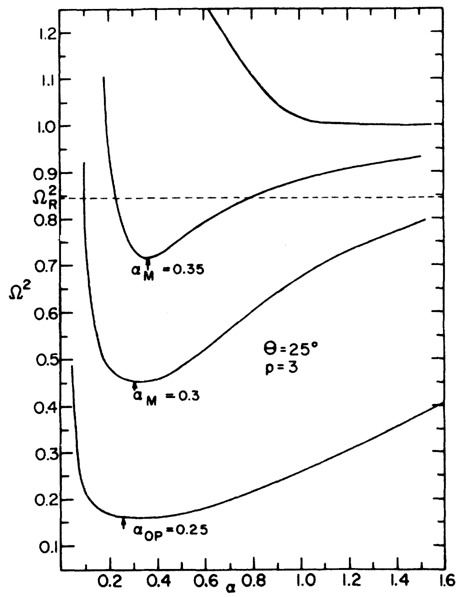

FIG. 1. Dependence of Γ_2-mode eigenvalues on the convergence factor α for a wedge angle of 25° for $p=3$.

$$A^{(33)}_{ij;kl}(m) = \frac{1}{\alpha^2}\{\text{Eq. (I25i)}\} + A(1-1/\alpha^2)\delta_{ik}\delta_{jl} \ . \quad \text{(3i)}$$

Use of Eqs. (3) in Eq. (I23) results in an eigenvalue matrix that may be diagonalized by standard numerical routines for nonsymmetric matrices to yield values for Ω^2.

Using the results given by Eq. (I23) and Eqs. (3), we have carried out calculations of eigenvalues for a number of wedge angles of less than 30°, for which convergence was found, in I, to be poor.

By choosing a small value of p, it was possible, by observing the dependence of the eigenvalues on α, to find an α which gave a minimum value for the lowest eigenvalue. We call this α_{op} (the optimum α). In Fig. 1 we have plotted the dependence of the three lowest eigenvalues on α for $p=3$ for a wedge angle of 25°. We note that for small p the minimum for higher eigenvalues occurs at a value of $\alpha(\alpha_M)$ different from α_{op}. We found, however, that as p was increased, α_M for higher eigenvalues decreased and approached α_{op} in the limit of large p. For these higher eigenvalues it is necessary both to increase p and adjust for a new α to give the best convergence. It should also be noted that

TABLE I. Values of the lowest Γ_2-mode eigenvalue for a 20°-angle wedge as a function of the number of terms retained in the expansion of the displacement amplitudes, obtained with the use of the appropriate convergence factor α_{op} and without the convergence factor ($\alpha = 1.0$).

p	Ω^2 with $\alpha_{op} = 0.20$	Ω^2 with $\alpha = 1.0$
1	0.111 459 56	0.478 380 22
2	0.110 683 04	0.304 969 66
3	0.110 677 85	0.220 359 77
4	0.110 677 83	0.174 695 20
5	0.110 677 83	0.148 539 52
6	0.110 677 83	0.133 058 86
7	0.110 677 83	0.123 775 43
8	0.110 677 83	0.118 217 79
9	0.110 677 83	0.114 931 59
10	0.110 677 83	0.113 025 77
11	0.110 677 83	0.111 945 82

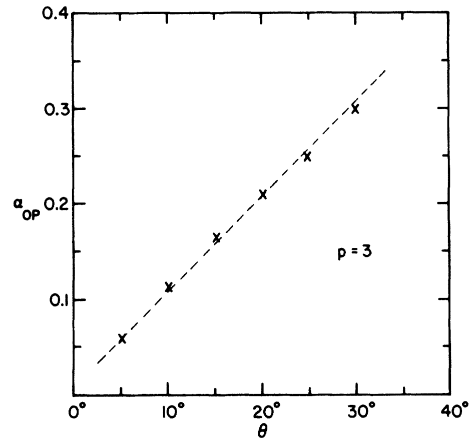

FIG. 2. Dependence of α_{op} for lowest Γ_2-mode eigenvalues on wedge angle θ for $p=3$. The dependence is nearly linear.

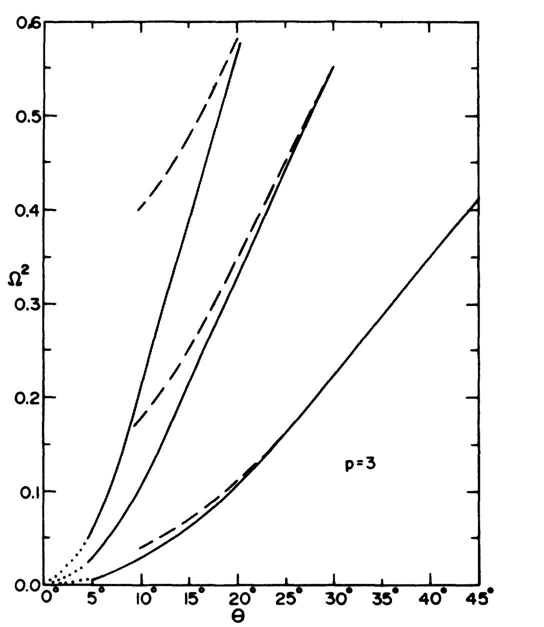

FIG. 3. Dependence on wedge angle θ of the lowest three eigenvalues for $p=3$. Dashed curves are results from I. Dotted portions of curves indicate extrapolations.

α_{op} for the lowest eigenvalue does not change as p is increased.

To illustrate the value of using α_{op}, we present in Table I the results for the lowest Γ_2-mode eigenvalue of a 20°-angle wedge. Using an α_{op} of 0.20, we obtained convergence to eight significant figures using only $p=4$, while with an α of 1.0 (no contribution from the convergence factor) convergence was not found, even out to $p=11$. A choice of $p=11$ gives a matrix of 156×156 to be diagonalized, whereas a choice of $p=4$ corresponds to a 30×30 matrix. The use of the convergence factor α not only gives far greater accuracy for small angles, but also yields a considerable savings in computational time.

In Fig. 2 we present the dependence of α_{op} for the lowest eigenvalue on the wedge angle θ. From Eq. (2) we see that the decrease in α_{op} as θ decreases indicates that the displacement pattern is more localized at the apex of the wedge as the wedge angle gets smaller.

Figure 3 summarizes the dependence of the lowest three eigenvalues on θ for angles less than 45°. These eigenvalues were calculated for $p=3$ and using α_{op} for the lowest eigenvalue. Consequently, the second and third lowest eigenvalue curves should be considered as being somewhat less precise than the lowest eigenvalue, although they are in error by less than 1%. We also show, in the same figure, for comparison the lowest three eigenvalues versus wedge angle as found in I for $p=12$ (a 182×182 matrix).

Thus, we have found that the use of a convergence factor enables us to obtain good results for Ω^2 using eigenvalue matrices very much smaller than those used in I.

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[1]S. L. Moss, A. A. Maradudin, and S. L. Cunningham, Phys. Rev. B (to be published).