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LATTICE THEORY OF FACE-SHEAR AND THICKNESS-TWIST WAVES IN F.C.C. CRYSTAL PLATES

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Abstract—Finite difference equations of motion of the sixth order and the associated boundary conditions for principal planes are formulated for a f.c.c. lattice of mass particles. The equations are solved for face-shear and thickness-twist waves in a plate with free faces. Computations of mode-shapes and the frequency spectrum are presented for copper and the results are compared with a previous solution for a simple cubic material and with the solution of the classical equations of elasticity.

1. INTRODUCTION

ONLY a few examples of lattice vibrational waves have been worked out for plates with free faces: Gazis and Wallis have examined the lowest mode of extensional motion [1] and the lowest mode of flexural motion [2] in an infinite plate of material with simple cubic symmetry and, for the same type of plate, Mindlin [3] has found the complete spectrum of face-shear and thickness-twist waves—i.e. waves with displacement and wave normal at right angles to each other and parallel to the faces of the plate. In all three examples, the difference equations of motion and boundary conditions employed were those formulated by Gazis *et al.* [4] for a simple cubic lattice in which account is taken of nearest and next nearest neighbor central force interactions and their special type of angular interaction between three non-collinear atoms. The purpose of the present paper is to describe the solution for f.c.c. crystals analogous to the problem solved by Mindlin [3] for the simple cubic case.

Equations of motion of a f.c.c. lattice, with two central force interactions and two angular interactions of the type introduced by Gazis *et al.* [4], have been formulated by Yuen and Varshni [5]. The central force interactions between nearest neighbor atoms [Fig. 1(a)] and between next nearest neighbor atoms [Fig. 1(b)] both lead to finite difference equations of motion of the fourth order; and the two angular interactions considered by Yuen and Varshni [Figs. 1(d) and 1(e)] also yield as high as, and only as high as, fourth order terms in the equations. There is a third angular interaction [Fig. 1(c)] which also contributes fourth order operators to the equations of motion and, furthermore, the sum of the distances between the three participating atoms is less than that for the angular interactions taken into account by Yuen and Varshni so that the additional angular interaction might be thought to be of importance. Nevertheless, when investigations were made of the effects of substituting this third angular interaction for the two considered by Yuen and Varshni and also of adding the third angular interaction to the Yuen and Varshni model, it was found that in the former case, the results were inferior to and, in the latter case, almost the same as

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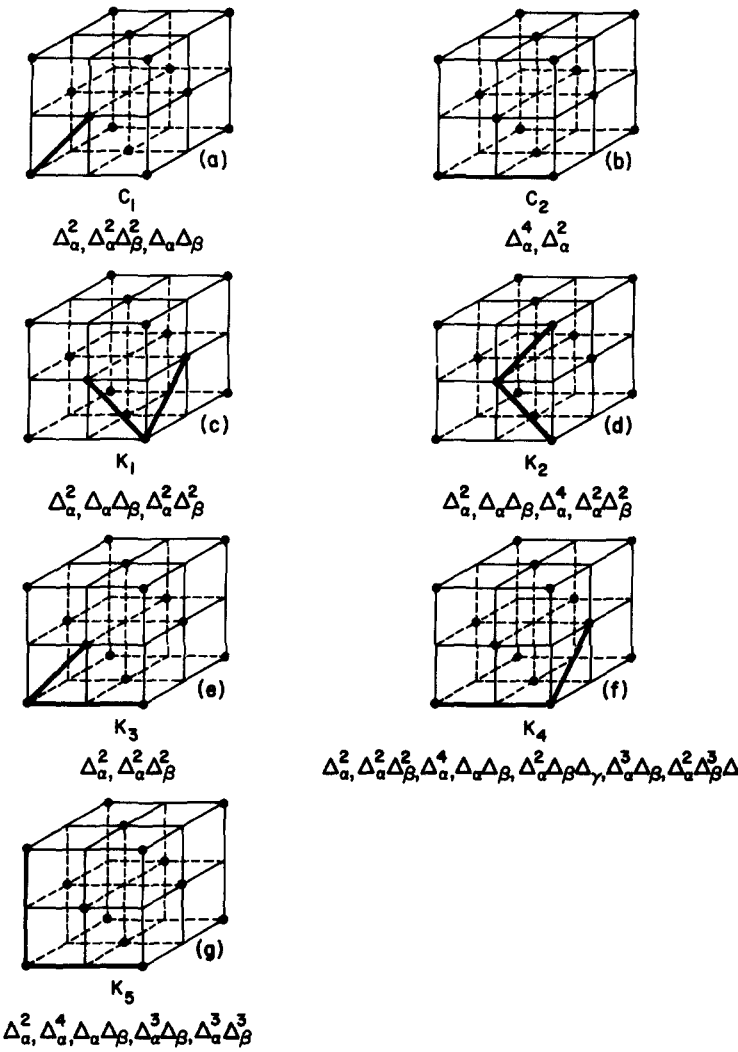

FIG. 1. Typical interactions and associated difference operators for a f.c.c. lattice.

those of Yuen and Varshni. These conclusions were based on the closeness of match obtainable between the computed dispersion curves for longitudinal and transverse bodily waves in the [100], [110] and [111] directions and those found from neutron diffraction measurements with copper by Svensson *et al.* [6], as shown in Fig. 2.

A further effort to improve the equations was somewhat more successful at little cost in additional complexity. Admission of sixth order difference operators, in the equations of motion, was found to require the addition of only two more angular interactions [Figs. 1(f) and 1(g)] and no further central force interactions. The resulting equations produced a small, but significant, improvement in the match with the Svensson *et al.* data, as shown in Fig. 2. These equations, along with the appropriate boundary conditions, were used to calculate

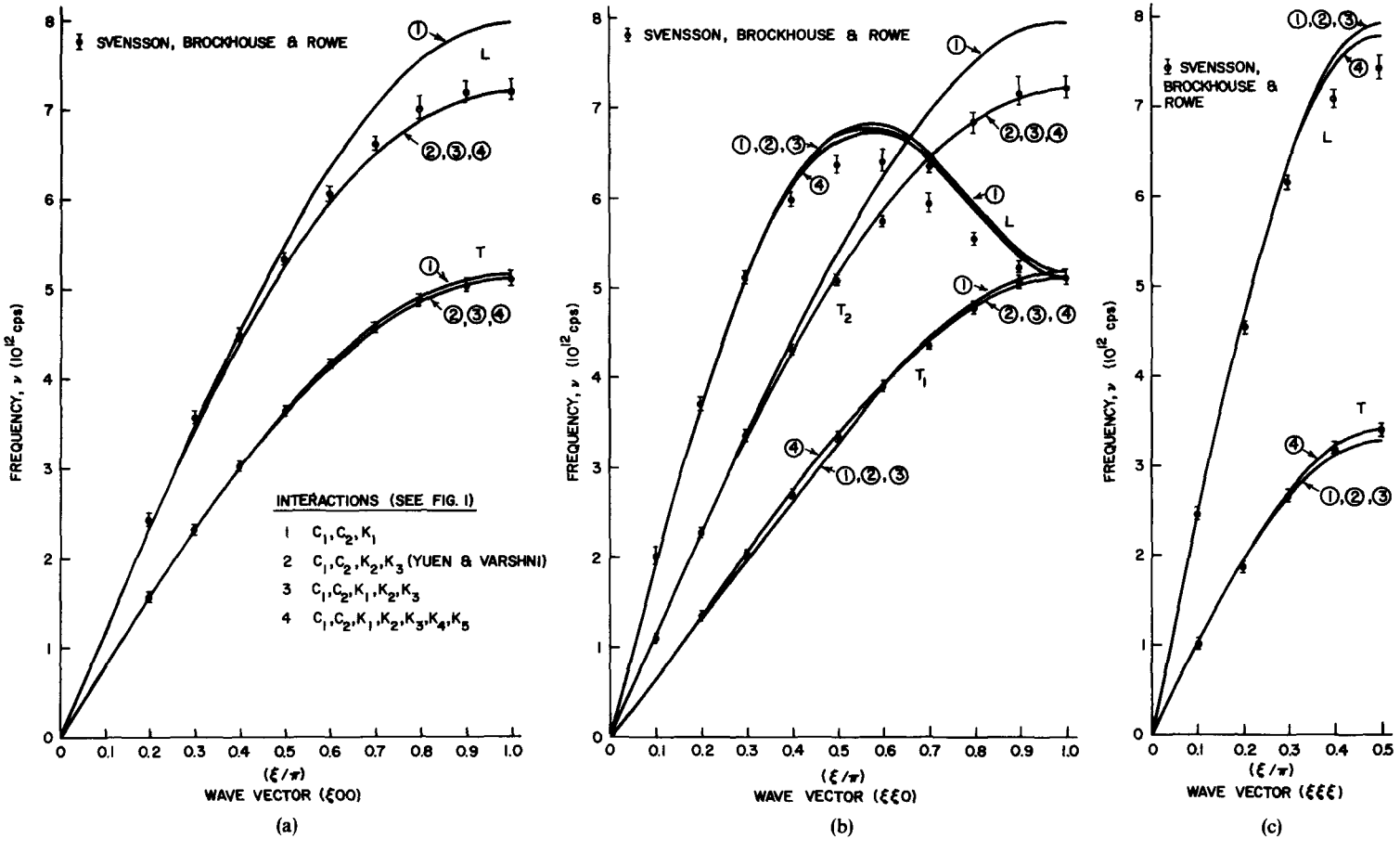

FIG. 2. The dispersion curves for copper at 296°K. The curves shown are theoretical ones obtained from the various angular force models. The experimental points are from Ref. [6].

the mode-shapes and complete frequency spectrum for a family of face-shear and thickness-twist waves with wave-normal and displacement in principal crystallographic directions in a plate bounded by principal crystallographic planes.

Although the solution for the plate of f.c.c. material is far more complicated than the one found by Mindlin [3] for the simple cubic case, the computed results are almost indistinguishable—although there are some qualitative differences of small magnitude. Accordingly, in general, the difference between the lattice solution and the solution based on the continuum theory of elasticity is about the same whether the lattice solution is for the simple cubic or the f.c.c. case.

Regarding the frequency spectrum (Fig. 4) there are as many real branches as there are layers of atoms across the thickness of the plate—in contrast to the infinity of branches in the continuum theory of elasticity. Each real branch has a low frequency cut-off at infinite wave length; but the cut-off frequencies are not integral multiples of the lowest, non-zero one, as they are in the continuum solution. As the wave length diminishes, each branch approaches a high frequency cut-off, whereas the frequencies in the continuum case approach infinity. The lattice frequencies are near the continuum frequencies only in the region where the wave lengths both along and across the plate are long in comparison with the distance between nearest neighbor atoms—i.e. in the lower left hand corner of Fig. 4. To the scale to which Fig. 4 is drawn, the difference between the spectra for simple cubic and f.c.c. is not noticeable.

As for mode-shapes across the thickness of the plate, the simple cubic and f.c.c. cases differ qualitatively. The displacements, in the former case, lie on sinusoids with real arguments; but, in the latter case, the displacements for each mode lie on a curve which is the sum of a sinusoid with a real argument and one with a complex argument, so that there are exponential parts (decaying inward from the surfaces). However, those parts are, comparatively, very small. At long wave lengths across the plate, the mode-shapes differ little from the continuum case, as illustrated in the lower portion of Fig. 5. However, the difference increases markedly as the wave length across the plate diminishes—i.e. as the order of the mode increases. Finally, whereas, in the simple cubic and continuum cases, the mode-shape across the thickness of the plate does not change, for a given order of mode, with change of wave length along the plate, there is a slight change in the f.c.c. case. This change, and also the difference between the simple cubic and f.c.c. mode-shapes, are not perceptible on the scale to which Fig. 5. is drawn.

2. FORCES ON A PARTICLE

Consider a f.c.c. lattice of identical particles of mass M. The particles occupy positions $(p_1a/2, p_2a/2, p_3a/2)$, denoted as P, where a is the lattice constant. The indices p_α, $\alpha = 1, 2, 3$ are integers with their sum always equal to an even integer. The potential energy of the lattice, U, is assumed to be:

$$U = U\{\Delta_{PQ}, \delta\theta_{PQR}\} \tag{1}$$

where Δ_{PQ} is the change in the distance between the particles at P and Q and $\delta\theta_{PQR}$ is the change in the angle whose vertex is at particle Q and whose arms extend to the particles at P and R.

The potential energy is expanded in a Taylor series about the equilibrium configuration, keeping only the harmonic terms:

$$U = \frac{1}{2}\sum_{Q,R} U(Q,R)\Delta_{QR}^2 + \frac{1}{2}\sum_{Q,R,S} U(Q,R,S)\delta\theta_{QRS}^2, \tag{2}$$

where

$$U(Q,R) = \frac{\partial^2 U}{\partial \Delta_{QR}^2} = U(R,Q), U(Q,R,S) = \frac{\partial^2 U}{\partial \delta\theta_{QRS}^2} = U(S,R,Q),$$

where the derivatives are evaluated at the equilibrium configuration. Then, if $\mathbf{U}_P$ is the displacement vector of particle P, the force on it is:

$$\mathbf{F}_P = \frac{-\partial U}{\partial \mathbf{U}_P} = -\sum_{Q,R} U(Q,R)\Delta_{QR}\frac{\partial \Delta_{QR}}{\partial \mathbf{U}_P} - \sum_{Q,R,S} U(Q,R,S)\delta\theta_{QRS}\frac{\partial \delta\theta_{QRS}}{\partial \mathbf{U}_P}, \tag{3}$$

where the first summation represents the central force terms and the second summation represents the angular force terms.

(a) *Central force terms*

Let the reference and deformed vectors extending from particle R to particle Q be $\mathring{\mathbf{r}}_{QR}$ and $\mathbf{r}_{QR}$ respectively. Then

$$\mathbf{r}_{QR} = \mathring{\mathbf{r}}_{QR} + \mathbf{U}_Q - \mathbf{U}_R \tag{4}$$

and

$$\Delta_{QR} = \Delta_{RQ} = |\mathbf{r}_{QR}| - |\mathring{\mathbf{r}}_{QR}|. \tag{5}$$

For displacements that are small compared to $\mathring{\mathbf{r}}_{QR}$,

$$\Delta_{QR} = \frac{\mathring{\mathbf{r}}_{QR}}{|\mathring{\mathbf{r}}_{QR}|} \circ (\mathbf{U}_Q - \mathbf{U}_R) \equiv \mathring{\mathbf{n}}_{QR} \circ (\mathbf{U}_Q - \mathbf{U}_R) \tag{6}$$

then

$$\frac{\partial \Delta_{QR}}{\partial \mathbf{U}_P} = \mathring{\mathbf{n}}_{QR}[\delta_{PQ} - \delta_{PR}]. \tag{7}$$

Now, due to the translational symmetry of the lattice, the coefficients $\mathbf{U}(P,Q)$ depend solely on the magnitude of the vector $\mathring{\mathbf{r}}_{PQ}$. Therefore, define:

$$h_\alpha = g_\alpha - p_\alpha, \alpha = 1,2,3, \mathbf{U}_Q - \mathbf{U}_P = \sum_{\alpha=1}^{3} \mathbf{e}_\alpha \lambda^\alpha_{h_1 h_2 h_3}, A(h_1 h_2 h_3) = 2U(Q,P)$$

then

$$\mathring{\mathbf{r}}_{QP} = \frac{a}{2}\sum_{\alpha=1}^{3} \mathbf{e}_\alpha h_\alpha$$

where $\mathbf{e}_\alpha$, $\alpha = 1, 2, 3$ are unit vectors parallel to the three axes of the cube. Then, the central force contribution to the force on particle P is:

$$\mathbf{F}_P = -\sum_{Q,R} U(Q,R)\Delta_{QR}\mathring{\mathbf{n}}_{QR}[\delta_{PQ}-\delta_{PR}] = 2\sum_{Q} U(Q,P)\Delta_{QP}\mathring{\mathbf{n}}_{QP},$$

$$= \sum_{h_1h_2h_3}\sum_{\alpha,\beta=1}^{3} \frac{A(h_1h_2h_3)\mathbf{e}_\beta h_\alpha h_\beta \lambda^\alpha_{h_1h_2h_3}}{(h_1^2+h_2^2+h_3^2)}. \tag{8}$$

This summation is continued over both positive and negative values of the indices h_1, h_2, h_3 up to some limiting value $H = (h_1^2+h_2^2+h_3^2)^{\frac{1}{2}}$, where $Ha/2$ is the limit on the distance between interacting particles. From the translational symmetry of the lattice, $A(h_1h_2h_3) = A(h_1h_2-h_3)$, etc. The summations over positive and negative values of the indices can therefore be replaced by summations over non-negative values. When this is done, the central force contribution to the force on particle P is:

$$\mathbf{F}_P = \sum_{h_1,h_2,h_3=0}^{H}\prod_{\varepsilon=1}^{3}(1-\tfrac{1}{2}\delta_{h_\varepsilon 0})\sum_{\alpha,\beta,\gamma=1}^{3} A(h_1h_2h_3)\mathbf{e}_\alpha[h_\alpha^2 \mathrm{O}_0(\lambda^\alpha_{h_1h_2h_3})+|e_{\alpha\beta\gamma}|h_\alpha h_\beta \mathrm{O}_\gamma(\lambda^\beta_{h_1h_2h_3})], \tag{9}$$

where $e_{\alpha\beta\gamma}$ is the alternator tensor,

$$\delta_{h_\alpha 0} = \begin{cases} 1 & h_{\alpha=0} \\ 0 & h_\alpha \neq 0 \end{cases}$$

and the difference operators are:

$$\begin{aligned}
\mathrm{O}_0(\lambda^\alpha_{h_1h_2h_3}) &= \lambda^\alpha_{h_1h_2h_3}+\lambda^\alpha_{h_1h_2-h_3}+\lambda^\alpha_{h_1-h_2h_3}+\lambda^\alpha_{h_1-h_2-h_3}+\lambda^\alpha_{-h_1h_2h_3}+\lambda^\alpha_{-h_1h_2-h_3}+\lambda^\alpha_{-h_1-h_2h_3} \\
&\quad +\lambda^\alpha_{h_1-h_2-h_3}, \\
\mathrm{O}_1(\lambda^\alpha_{h_1h_2h_3}) &= \lambda^\alpha_{h_1h_2h_3}+\lambda^\alpha_{-h_1h_2h_3}+\lambda^\alpha_{h_1-h_2-h_3}+\lambda^\alpha_{-h_1-h_2-h_3}-\lambda^\alpha_{h_1h_2-h_3}-\lambda^\alpha_{-h_1h_2-h_3}-\lambda^\alpha_{h_1-h_2h_3} \\
&\quad -\lambda^\alpha_{-h_1-h_2h_3}, \\
\mathrm{O}_2(\lambda^\alpha_{h_1h_2h_3}) &= \lambda^\alpha_{h_1h_2h_3}+\lambda^\alpha_{h_1-h_2h_3}+\lambda^\alpha_{-h_1h_2-h_3}+\lambda^\alpha_{-h_1-h_2-h_3}-\lambda^\alpha_{h_1h_2-h_3}-\lambda^\alpha_{h_1-h_2-h_3}-\lambda^\alpha_{-h_1h_2h_3} \\
&\quad -\lambda^\alpha_{-h_1-h_2h_3}, \\
\mathrm{O}_3(\lambda^\alpha_{h_1h_2h_3}) &= \lambda^\alpha_{h_1h_2h_3}+\lambda^\alpha_{h_1h_2-h_3}+\lambda^\alpha_{-h_1-h_2h_3}+\lambda^\alpha_{-h_1-h_2-h_3}-\lambda^\alpha_{h_1-h_2h_3}-\lambda^\alpha_{h_1-h_2-h_3}-\lambda^\alpha_{-h_1h_2h_3} \\
&\quad -\lambda^\alpha_{-h_1h_2-h_3}.
\end{aligned} \tag{10}$$

(b) *Angular force terms*

Let the angles formed at particle R by the vectors extending from R to the particles at Q and S be $\mathring{\theta}_{QRS}$ and θ_{QRS} in the reference and deformed states respectively, with $\theta_{QRS} = \mathring{\theta}_{QRS}+\delta\theta_{QRS}$. Then, for $|\delta\theta_{QRS}| \ll 1$, and for displacements small compared to the reference vectors,

$$\begin{aligned}
\delta\theta_{QRS} &= (\cos\mathring{\theta}_{QRS}-\cos\theta_{QRS})/\sin\mathring{\theta}_{QRS} \\
&= \{\mathbf{U}_R\circ[\mathring{\mathbf{r}}_{QR}+\mathring{\mathbf{r}}_{SR}-(\mathring{\mathbf{n}}_{QR}|\mathring{\mathbf{r}}_{SR}|+\mathring{\mathbf{n}}_{SR}|\mathring{\mathbf{r}}_{QR}|)(\mathring{\mathbf{n}}_{QR}\circ\mathring{\mathbf{n}}_{SR})]-\mathbf{U}_Q\circ[\mathring{\mathbf{r}}_{SR}-\mathring{\mathbf{n}}_{QR}|\mathring{\mathbf{r}}_{SR}|(\mathring{\mathbf{n}}_{SR}\circ\mathring{\mathbf{n}}_{QR})] \\
&\quad -\mathbf{U}_S\circ[\mathring{\mathbf{r}}_{QR}-\mathring{\mathbf{n}}_{SR}|\mathring{\mathbf{r}}_{QR}|(\mathring{\mathbf{n}}_{SR}\circ\mathring{\mathbf{n}}_{QR})]\}/|\mathring{\mathbf{r}}_{QR}\times\mathring{\mathbf{r}}_{SR}|
\end{aligned} \tag{11}$$

for $\mathring{\theta}_{QRS} \neq 0, \Pi$. Then

$$\begin{aligned}
\frac{\partial\delta\theta_{QRS}}{\partial\mathbf{U}_P} &= \{\delta_{RP}[\mathring{\mathbf{r}}_{QR}+\mathring{\mathbf{r}}_{SR}-(\mathring{\mathbf{n}}_{QR}|\mathring{\mathbf{r}}_{SR}|+\mathring{\mathbf{n}}_{SR}|\mathring{\mathbf{r}}_{QR}|)(\mathring{\mathbf{n}}_{QR}\circ\mathring{\mathbf{n}}_{SR})]-\delta_{QP}[\mathring{\mathbf{r}}_{SR}-\mathring{\mathbf{n}}_{QR}|\mathring{\mathbf{r}}_{SR}|(\mathring{\mathbf{n}}_{QR}\circ\mathring{\mathbf{n}}_{SR})] \\
&\quad -\delta_{SP}[\mathring{\mathbf{r}}_{QR}-\mathring{\mathbf{n}}_{SR}|\mathring{\mathbf{r}}_{QR}|(\mathring{\mathbf{n}}_{SR}\circ\mathring{\mathbf{n}}_{QR})]\}/|\mathring{\mathbf{r}}_{QR}\times\mathring{\mathbf{r}}_{SR}|.
\end{aligned} \tag{12}$$

The angular force contribution to the force on particle P is then:

$$\mathbf{F}_P = -\sum_{Q,S} U(Q,P,S)\delta\theta_{QPS}[\mathring{\mathbf{r}}_{QP}+\mathring{\mathbf{r}}_{SP}-(\mathring{\mathbf{n}}_{QP}|\mathring{\mathbf{r}}_{SP}|+\mathring{\mathbf{n}}_{SP}|\mathring{\mathbf{r}}_{QP}|)(\mathring{\mathbf{n}}_{QP}\circ\mathring{\mathbf{n}}_{SP})]/|\mathring{\mathbf{r}}_{QP}\times\mathring{\mathbf{r}}_{SP}|$$

$$+\sum_{R,S} U(P,R,S)\delta\theta_{PRS}[\mathring{\mathbf{r}}_{SR}-\mathring{\mathbf{n}}_{PR}|\mathring{\mathbf{r}}_{SR}|(\mathring{\mathbf{n}}_{PR}\circ\mathring{\mathbf{n}}_{SR})]/|\mathring{\mathbf{r}}_{SR}\times\mathring{\mathbf{r}}_{PR}|$$

$$+\sum_{Q,R} U(Q,R,P)\delta\theta_{QRP}[\mathring{\mathbf{r}}_{QR}-\mathring{\mathbf{n}}_{PR}|\mathring{\mathbf{r}}_{QR}|(\mathring{\mathbf{n}}_{PR}\circ\mathring{\mathbf{n}}_{QR})]/|\mathring{\mathbf{r}}_{QR}\times\mathring{\mathbf{r}}_{PR}|. \tag{13}$$

Now, due to the translational symmetry of the lattice, the coefficients $U(Q,R,S)$ depend only on the magnitudes and relative orientations of the vectors $\mathring{\mathbf{r}}_{QR}$ and $\mathring{\mathbf{r}}_{SR}$. This dependence may be expressed as

$$U(Q,R,S) = U(Q,R,S)\{|\mathring{\mathbf{r}}_{QR}|,|\mathring{\mathbf{r}}_{SR}|,(\mathring{\mathbf{r}}_{QR}\circ\mathring{\mathbf{r}}_{SR})\}. \tag{14}$$

Therefore, in the summations above, employ the following definitions:

first summation	second summation
$h_\alpha = q_\alpha - p_\alpha,\ h'_\alpha = s_\alpha - p_\alpha$	$h_\alpha = r_\alpha - p_\alpha,\ h'_\alpha = r_\alpha - s_\alpha,\ j_\alpha = h'_\alpha - h_\alpha$
$\mathrm{A}^{(h_1h_2h_3)}_{h'_1h'_2h'_3} = U(Q,P,S)$	$\mathrm{A}^{(h_1h_2h_3)}_{h'_1h'_2h'_3} = A^{(-h_1-h_2-h_3)}_{-h'_1-h'_2-h'_3} = U(P,R,S)$

third summation

$$h_\alpha = r_\alpha - q_\alpha,\ h'_\alpha = r_\alpha - p_\alpha, j_\alpha = h'_\alpha - h_\alpha$$
$$A^{(h_1h_2h_3)}_{h'_1h'_2h'_3} = A^{(-h_1-h_2-h_3)}_{-h'_1-h'_2-h'_3} = U(Q,R,P,)$$

then

$$\mathring{\mathbf{r}}_{QP} = (a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h_\alpha \qquad \mathring{\mathbf{r}}_{PR} = -(a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h_\alpha \qquad \mathring{\mathbf{r}}_{QR} = -(a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h_\alpha$$

$$\mathring{\mathbf{r}}_{SP} = (a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h'_\alpha \qquad \mathring{\mathbf{r}}_{SR} = -(a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h'_\alpha. \qquad \mathring{\mathbf{r}}_{PR} = -(a/2)\sum_{\alpha=1}^{3}\mathbf{e}_\alpha h'_\alpha.$$

Then, the angular force contribution to the force on particle P is:

$$\mathbf{F}_P = \sum_{\substack{h_1h_2h_3\\ h'_1h'_2h'_3}}^{H}\sum_{\alpha,\beta=1}^{3} A^{(h_1h_2h_3)}_{h'_1h'_2h'_3}\mathbf{e}_\alpha\{(a_\alpha+a'_\alpha)(a_\beta\lambda^\beta_{h_1h_2h_3}+a'_\beta\lambda^\beta_{h'_1h'_2h'_3})+(a_\beta+a'_\beta)(a_\alpha\lambda^\beta_{h_1h_2h_3}+a'_\alpha\lambda^\beta_{h'_1h'_2h'_3})$$
$$-(a'_\alpha a_\beta\lambda^\beta_{j_1j_2j_3}+a_\alpha a'_\beta\lambda^\beta_{-j_1-j_2-j_3})\}/(a/2)^2(\sigma\sigma')^2(\sigma\sigma'-\tau^2) \tag{15}$$

where

$$\sigma = \sum_{\alpha=1}^{3} h_\alpha^2,\ \sigma' = \sum_{\alpha=1}^{3} h_\alpha'^2,\ \tau = \sum_{\alpha=1}^{3} h_\alpha h'_\alpha,\ a_\alpha = (h'_\alpha\sigma - h_\alpha\tau)\sigma',\ a'_\alpha = (h_\alpha\sigma' - h'_\alpha\tau)\sigma,\ \alpha = 1,2,3.$$

From the definition of the $A^{(h_1h_2h_3)}_{(h_1'h_2'h_3')}$ and equation (14) it is easily shown that $A^{(h_1h_2h_3)}_{(h_1'h_2'h_3')} = A^{(h_1h_2-h_3)}_{(h_1'h_2'-h_3')}$, etc. Using this, the double summations on the indices h_α, h_α' over both positive and negative values can be replaced by summations over non-negative values. First define:

$$M^{(h_1h_2h_3)}_{(h_1'h_2'h_3')} = \sum_{\alpha,\beta,\gamma=1}^{3} \mathbf{e}_\alpha[[2(a_\alpha+a_\alpha')[a_\alpha O_0(\lambda^\alpha_{h_1h_2h_3})+a_\alpha' O_0(\lambda^\alpha_{h_1'h_2'h_3'})]-2a_\alpha a_\alpha' O_0(\lambda^\alpha_{j_1j_2j_3})$$
$$+|e_{\alpha\beta\gamma}|\{[a_\gamma(a_\alpha+a_\alpha')+a_\alpha(a_\gamma+a_\gamma')]O_\beta(\lambda^\alpha_{h_1h_2h_3})+[a_\gamma'(a_\alpha+a_\alpha')+a_\alpha'(a_\gamma+a_\gamma')]O_\beta(\lambda^\gamma_{h_1'h_2'h_3'})$$
$$-(a_\alpha' a_\gamma+a_\alpha a_\gamma')O_\beta(\lambda^\gamma_{j_1j_2j_3})\}]]/(a/2)^2(\sigma\sigma'-\tau^2),$$

then employing the convention:

$$A^{(h_1h_2h_3}_{(h_1'h_2'\pm h_3'}M^{(h_1h_2h_3}_{(h_1'h_2'\pm h_3'} = A^{(h_1h_2h_3)}_{(h_1'h_2'h_3'}M^{(h_1h_2h_3)}_{(h_1'h_2'h_3'}+A^{(h_1h_2h_3}_{(h_1'h_2'-h_3'}M^{(h_1h_2h_3}_{(h_1'h_2'-h_3'},$$

etc., the angular force contribution to the force on particle P is:

$$\mathbf{F}_P = \prod_{\alpha=1}^{3}[1-(\delta_{h_\alpha 0}+\delta_{h_\alpha' 0})/2+\delta_{h_\alpha h_\alpha' 0}/4] \sum_{\substack{h_1,h_2,h_3=0\\ h_1',h_2',h_3'=0}}^{H} A^{(h_1h_2h_3}_{\pm h_1'\pm h_2'\pm h_3'}M^{(h_1h_2h_3}_{\pm h_1'\pm h_2'\pm h_3'}, \tag{16}$$

where

$$\delta_{h_\alpha h_\alpha' 0} = \begin{cases} 1 & h_\alpha = h_\alpha' = 0 \\ 0 & \text{otherwise} \end{cases}$$

3. BOUNDARY CONDITIONS

A free boundary is formed by the removal of all particles on one side ($p_1 < 0$) of the layer $p_1 = 0$. The boundary conditions state that the sum of all forces on a particle, which arise from interaction with any of the removed particles, is zero.

(a) *Central force terms*

The boundary conditions on the central force contributions are obtained from equation (8) by restricting the summation over index h_1 to $h_1 + p_1 < 0$ and setting the result equal to zero. This restriction has no effect on the summations over the indices h_2, h_3; so, after proceeding in a manner similar to that used to obtain equation (9), the result is:

$$0 = \sum_{h_1+p_1<0}\sum_{h_2,h_3=0}^{H}\prod_{\varepsilon=1}^{3}(1-\delta_{h_\varepsilon 0}/2)\sum_{\alpha,\beta,\gamma=1}^{3} A(h_1h_2h_3)\mathbf{e}_\alpha[h_\alpha^2\bar{O}_0(\lambda^\alpha_{h_1h_2h_3})+|e_{\alpha\beta\gamma}|h_\alpha h_\beta\bar{O}_\gamma(\lambda^\beta_{h_1h_2h_3})]$$
$$\div(h_1^2+h_2^2+h_3^2), \tag{17}$$

where the operators $\bar{O}_\gamma(\lambda^\alpha_{h_1h_2h_3})$ are obtained from the operators $O_\gamma(\lambda^\alpha_{h_1h_2h_3})$, equation (10) by setting $\lambda^\alpha_{-h_1h_2h_3} = \lambda^\alpha_{-h_1h_2-h_3} = \lambda^\alpha_{-h_1-h_2h_3} = \lambda^\alpha_{-h_1-h_2-h_3} = 0$.

(b) *Angular force terms*

The boundary condition on the angular force contributions is obtained from equation (13) by restricting the summations over h_1 and h_1' to cases where one or both of the particles in the interaction have been removed and setting the sum equal to zero. The summations over the indices h_2, h_2', h_3, h_3' are unaffected by the restrictions placed on the summations

over h_1 and h_1'. Each of the three summations in equation (13) yields three sums contributing to the boundary conditions: in each of the first two contributions, one of the interacting particles, Q or S, R or S, Q or R has been removed, in the third contribution both particles have been removed. Employing the same definitions as previously, the angular force contribution to the boundary conditions is:

$$0 = \sum_{h_1' < -p_1} \sum_{h_1} A'\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'}[\bar{M}\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} + M^*\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'}]$$
$$+ \sum_{h_1 < -p_1} \sum_{h_1'} A'\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} M^*\binom{h_1' \pm h_2' \pm h_3'}{h_1 h_2 h_3} + \sum_{h_1 \geq -p_1} \sum_{h_1' > p_1 + h_1} A'\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} M^*\binom{h_1' \pm h_2' \pm h_3'}{h_1 h_2 h_3}$$
$$+ \sum_{h_1' \geq -p_1} \sum_{h_1 > p_1 + h_1} A'\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} M^*\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} + \sum_{h_1 < p_1} \sum_{h_1' \geq -p_1} A'\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'} \bar{M}\binom{h_1 h_2 h_3}{h_1' \pm h_2' \pm h_3'}, \tag{18}$$

where

$$A'\binom{h_1 h_2 h_3}{h_1' h_2' h_3'} = A\binom{h_1 h_2 h_3}{h_1' h_2' h_3'} \prod_{\alpha=2}^{3} [1 - (\delta_{h_\alpha 0} + \delta_{h_\alpha' 0})/2 + \delta_{h_\alpha h_\alpha' 0}/4],$$

$$\bar{M}\binom{h_1 h_2 h_3}{h_1' h_2' h_3'} = \sum_{\alpha,\beta,\gamma=1}^{3} \mathbf{e}_\alpha (a_\alpha + a_\alpha')\{a_\alpha \bar{O}_0(\lambda^\alpha_{h_1 h_2 h_3}) + a_\alpha' \bar{O}_0(\lambda^\alpha_{h_1' h_2' h_3'}) + |e_{\alpha\beta\gamma}|[a_\gamma \bar{O}_\beta(\lambda^\gamma_{h_1' h_2' h_3'})$$
$$+ a_\gamma' \bar{O}_\beta(\lambda^\gamma_{h_1' h_2' h_3'})]\}/(a/2)^2(\sigma\sigma')^2(\sigma\sigma' - \tau^2),$$

$$M^*\binom{h_1 h_2 h_3}{h_1' h_2' h_3'} = \sum_{\alpha,\beta,\gamma=1}^{3} \mathbf{e}_\alpha a_\alpha' \{(a_\alpha + a_\alpha')\bar{O}_0(\lambda^\alpha_{h_1' h_2' h_3'}) - a_\alpha \bar{O}_0(\lambda^\alpha_{j_1 j_2 j_3}) + |e_{\alpha\beta\gamma}|[(a_\gamma + a_\gamma')\bar{O}_\beta(\lambda^\gamma_{h_1' h_2' h_3'})$$
$$- a_\gamma \bar{O}_\beta(\lambda^\gamma_{j_1 j_2 j_3})]\}/(a/2)^2(\sigma\sigma')^2(\sigma\sigma' - \tau^2).$$

Adding expressions (17) and (18) yields the boundary conditions on the boundary layers $p_1 = 0, 1, 2, \ldots$.

4. DIFFERENCE OPERATORS

For a function

$$\mathbf{F}_P \equiv F\left\{\frac{a}{2}(\mathbf{e}_1 p_1 + \mathbf{e}_2 p_2 + \mathbf{e}_3 p_3)\right\} \equiv F(p),$$

define the differences:

$$\Delta_\alpha^+ F_P = F(P + \mathbf{e}_\alpha) - F(P) \qquad \Delta_\alpha^- F_P = F(P) - F(P - \mathbf{e}_\alpha)$$
$$E_\alpha F_P = F(P + \mathbf{e}_\alpha) \qquad \bar{E}_\alpha F_P = F(P - \mathbf{e}_\alpha)$$
$$\Delta_\alpha^2 F_P = \Delta_\alpha^+ \Delta_\alpha^- F_P \qquad \Delta_\alpha F_P = \tfrac{1}{2}(\Delta_\alpha^+ + \Delta_\alpha^-) F_P \qquad \alpha = 1, 2, 3.$$

Then

$$\lambda^\alpha_{h_1 h_2 h_3} = U^\alpha_{p_1 + h_1, p_2 + h_2, p_3 + h_3} - U^\alpha_{p_1, p_2, p_3} = (E_1^{h_1} E_2^{h_2} E_3^{h_3} - I) U^\alpha_{p_1 p_2 p_3} \tag{19}$$

where $E_\alpha^2 F_P = E_\alpha(E_\alpha F_P)$, etc. and I is the operator identity symbol. These expressions are substituted for the terms in the difference operators equation (10), and the results expanded. The general expressions for the results are given in the Appendix; for the present work,

however, the restrictions $h_\alpha \leq 3$, $\alpha = 1, 2, 3$ have been imposed, which yield the expressions:

$$O_0(\lambda^\alpha_{h_1h_2h_3}) = \left\{ \prod_{\beta=1}^{3} [2 + h_3^2\Delta_\beta^2 + (\delta_{h_\beta 2} + 6\delta_{h_\beta 3})\Delta_\beta^4 + \delta_{h_\beta 3}\Delta_\beta^6] - 8 \right\} U^\alpha_{p_1p_2p_3}$$

$$O_1(\lambda^\alpha_{h_1h_2h_3}) = 4\Big\{ [2 + h_1^2\Delta_1^2 + (\delta_{h_1 2} + 6\delta_{h_1 3})\Delta_1^4 + \delta_{h_1 3}\Delta_1^6] \prod_{\beta=2}^{3} [h_\beta\Delta_\beta + (\delta_{h_\beta 2} + 4\delta_{h_\beta 3})\Delta_\beta^2\Delta_\beta + \delta_{h_\beta 3}\Delta_\beta^4\Delta_\beta] \Big\} U^\alpha_{p_1p_2p_3}$$

$$O_2(\lambda^\alpha_{h_1h_2h_3}) = 4\Big\{ [2 + h_2^2\Delta_2^2 + (\delta_{h_2 2} + 6\delta_{h_2 3})\Delta_2^4 + \delta_{h_2 3}\Delta_2^6] \prod_{\beta=1,3}^{3} [h_\beta\Delta_\beta + (\delta_{h_\beta 2} + 4\delta_{h_\beta 3})\Delta_\beta^2\Delta_\beta + \delta_{h_\beta 3}\Delta_\beta^4\Delta_\beta] \Big\} U^\alpha_{p_1p_2p_3}$$

$$O_3(\lambda^\alpha_{h_1h_2h_3}) = 4\Big\{ [2 + h_3^2\Delta_3^2 + (\delta_{h_3 2} + 6\delta_{h_3 3})\Delta_3^4 + \delta_{h_3 3}\Delta_3^6] \prod_{\beta=1}^{2} [h_\beta\Delta_\beta + (\delta_{h\beta 2} + 4\delta_{h_\beta 3})\Delta_\beta^2\Delta_\beta + \delta_{h_\beta 3}\Delta_\beta^4\Delta_\beta] \Big\} U^\alpha_{p_1p_2p_3}.$$

5. INTERACTIONS PRESENT

We wish to consider a model which contains all central and angular interactions that give rise to finite difference equations of motion of order not higher than 2K, where K is some positive integer. Any interaction which would lead to finite differences of an order higher than 2K in the equations of motion is eliminated from consideration. The finite differences appearing in the equations of motion due to each interaction are expressed in terms of the difference operators $O_\alpha(\lambda^\beta_{h_1h_2h_3})$ by equations (8) and (16). These difference operators are expressed in terms of central differences by equation (10). The highest order central differences that appear in the operators $O_\alpha(\lambda^\beta_{h_1h_2h_3})$ are: in $O_0(\lambda^\beta_{h_1h_2h_3})$ the order of the highest difference is $2(h_1+h_2+h_3)$; in $O_\alpha(\lambda^\beta_{h_1h_2h_3})$, $\alpha = 1, 2, 3$, this order is $2(h_1+h_2+h_3-1)$. The restriction that any interaction considered shall give rise to differences of orders $\leq 2K$ requires that $h_1+h_2+h_3 \leq K$, unless the coefficients of $O_0(\lambda^\beta_{h_1h_2h_3})$ in the equations of motion vanish. If this is so, the restriction requires $h_1+h_2+h_3 \leq K+1$. The coefficients of $O_0(\lambda^\beta_{h_1h_2h_3})$ for the central and angular force contributions will now be investigated.

For the central force contribution to the force on a particle, equation (9) shows that the $\mathbf{e}_\alpha$ component of the force contains the term $h_\alpha^2 O_0(\lambda^\alpha_{h_1h_2h_3})$. The requirement that this term vanishes for $\alpha = 1, 2, 3$ results in a particle interacting with itself. Therefore, for the central force interactions considered, $h_1+h_2+h_3 \leq K$.

For the angular force contribution to the force on a particle, equation (16) shows that the $\mathbf{e}_\alpha$ component of the force contains the terms $a_\alpha(a_\alpha+a'_\alpha)O_0(\lambda^\alpha_{h_1h_2h_3})$, $\alpha'_\alpha + a_\alpha O_0(\lambda^\alpha_{h'_1h'_2h'_3})$ and $a_\alpha a'_\alpha O_0(\lambda^\alpha_{j_1j_2j_3})$. Since the first term becomes identical to the second under an interchange of indices, it is sufficient to examine only the first and third terms.

The requirement that the first term vanishes for $\alpha = 1, 2, 3$ yields, when summed over α:

$$\sigma\sigma'(\sigma' - J)(\sigma\sigma' - \tau^2) = 0$$

but $\sigma\sigma'(\sigma\sigma' - J^2) \neq 0$, since it is assumed that there are three non-collinear particles in the angular interaction. There remains $\sigma' = \tau$, then

$$a_1(a_1 + a'_1) = (\sigma - \sigma')\tau^2 h_1(h'_1\sigma - h_1\sigma'_1) = 0.$$

The possibilities are:

1. $\sigma = \sigma'$, but then $\sigma\sigma' - \tau^2 = 0$, which is not possible;
2. $h_1 = 0$, but cyclical permutation gives $h_2 = h_3 = 0$, which is not possible;
3. $\tau = 0$, but then $\sigma' = 0$, which is not possible;
4. $h_1'\sigma - h_1\sigma' = 0$ or $h_1' = h_1\sigma'/\sigma$; but cyclical permutation gives $h_2' = h_2\sigma'/\sigma$, $h_3' = h_3\sigma'/\sigma$, which lead to $\sigma\sigma' - \tau^2 = 0$ which is not possible.

The result is that it is impossible to satisfy the requirement that the term $a_\alpha(a_\alpha + a_\alpha')$ $\times O_0(\lambda^\alpha_{h_1h_2h_3})$ vanishes for $\alpha = 1, 2, 3$. Therefore, for the angular force interactions considered $h_1 + h_2 + h_3 \leq K$, and on account of the symmetry noted above, $h_1' + h_2' + h_3' \leq K$.

The requirement that the third term vanishes for $\alpha = 1, 2, 3$ yields, when summed over α:

$$\sigma\sigma'\tau(\sigma\sigma' - \tau^2) = 0$$

which is possible only if $\tau = 0$. With this, the requirement is that $h_1h_1' = h_2h_2' = h_3h_3' = 0$. It is therefore possible to have interactions for which $j_1 + j_2 + j_3 = K + 1$ if $h_\alpha h_\alpha' = 0$, $\alpha = 1, 2, 3$.

Consider a model of a f.c.c. lattice for which $K = 3$, i.e. a model containing all the interactions which lead to sixth order difference equations of motion. From the above considerations, the only possible values for the indices h_α, h_α' in the central and angular force interactions are the permutations of (110) and (200). The possible combinations for the angular interactions are presented in Table 1, and the interactions considered are noted.

TABLE 1. COMBINATIONS OF THE INDICES (h_1, h_2, h_3), (h_1', h_2', h_3') WITH THE ANGULAR INTERACTIONS PRESENT AND THE CORRESPONDING FORCE CONSTANTS

$h_1h_2h_3$	$h_1'h_2'h_3'$	$j_1j_2j_3$	τ	Comments	Force constants
1 1 0	1 1 0	0 0 0	2	Omitted, particle interacts with itself	
1 1 0	0 1 1	−1 0 1	1	Retained	$K_1 = 4A\binom{110}{011}$
1 1 0	1 −1 0	0 −2 0	0	Retained	$K_2 = 4A\binom{110}{1-10}$
1 1 0	0 −1 1	−1 −2 1	−1	Omitted, $\lvert j_1\rvert + \lvert j_2\rvert + \lvert j_3\rvert = 4, \tau \neq 0$	
1 1 0	−1 −1 0	−2 −2 0	−2	Omitted, $\lvert j_1\rvert + \lvert j_2\rvert + \lvert j_3\rvert = 4, \tau \neq 0$	
1 1 0	2 0 0	1 −1 0	2	Retained	$K_3 = 2A\binom{110}{200}$
1 1 0	0 0 2	−1 −1 2	0	Retained	$K_4 = 2A\binom{110}{002}$
1 1 0	−2 0 0	−3 −1 0	−2	Omitted, $\lvert j_1\rvert + \lvert j_2\rvert + \lvert j_3\rvert = 4, \tau \neq 0$	
2 0 0	2 0 0	0 0 0	4	Omitted, particle interacts with itself	
2 0 0	0 2 0	−2 2 0	0	Retained	$K_5 = 4A\binom{200}{020}$
2 0 0	−2 0 0	−4 0 0	−4	Omitted, $\lvert j_1\rvert + \lvert j_2\rvert + \lvert j_3\rvert = 4, \tau \neq 0$	

There are therefore seven interactions considered: two central force, with coefficients $A(110)$, $A(200)$, and five angular, with coefficients $A\binom{110}{011}$, $A\binom{110}{1-10}$, $A\binom{110}{200}$, $A\binom{110}{002}$, $A\binom{200}{020}$. These coefficients may be related to the central and angular force constants. For the central force constants C_j, $j = 1, 2$, using equation (3) and the fact that $\Delta_{PQ} = \Delta_{QP}$ yields

$$C_1 = A(110), \qquad C_2 = A(200).$$

A similar argument holds for the angular force coefficients if an additional factor is introduced in the instances where the summation over the indices counts an angle more than once. The method employed was to consider every permutation of the indices $(h_1h_2h_3)$,

combining each permutation with all possible combinations of the indices $(\pm h'_1 \pm h'_2 \pm h'_3)$ consistent with the particular angular interaction. For the instances in which the indices $(h'_1 h'_2 h'_3)$ are some rearrangement of the indices $(h_1 h_2 h_3)$ this method counts each angular interaction twice. Consequently, in these instances an additional factor of two is introduced in the relationship between the force constants K_j, $j = 1, \ldots, 5$, and the coefficients $A^{(h_1 h_2 h_3)}_{(h'_1 h'_2 h'_3)}$. These relationships are summarized in Table 1.

Typical illustrations of the particles participating in each of the seven interactions are shown in Fig. 1.

6. EQUILIBRIUM EQUATIONS, BOUNDARY CONDITIONS

Substituting the values of the indices, for the interactions considered, into equations (9) and (16) yields the equilibrium equations:

$$\begin{aligned} M\ddot{U}^1_{p_1p_2p_3} = {} & B_1 O_0(\lambda^1_{110} + \lambda^1_{101}) + B_2 O_0(\lambda^1_{011}) + B_3[O_3(\lambda^2_{110}) + O_2(\lambda^3_{101})] + B_4 O_0(\lambda^1_{200}) \\ & + B_5 O_0(\lambda^1_{020} + \lambda^1_{002}) + B_6[O_2(\lambda^3_{211} + \lambda^3_{121}) + O_3(\lambda^2_{211} + \lambda^2_{112})] \\ & + B_7[O_3(\lambda^2_{220}) + O_2(\lambda^3_{202})], \end{aligned} \tag{20}$$

or, with the difference operators expanded,

$$\begin{aligned} M\ddot{U}^1_{p_1p_2p3} = {} & [b_1\Delta_1^2 + b_2(\Delta_2^2 + \Delta_3^2) + b_3\Delta_1^4 + b_4\Delta_1^2(\Delta_2^2 + \Delta_3^2) + b_5(\Delta_2^4 + \Delta_3^4) + b_6\Delta_2^2\Delta_3^2]U^1_{p_1p_2p_3} \\ & + [b_7\Delta_3^2 + b_9(\Delta_1^2 + \Delta_2^2) + b_{10}\Delta_3^2(\Delta_1^2 + \Delta_2^2) + b_{11}\Delta_1^2\Delta_2^2]\Delta_1\Delta_2 U^2_{p_1p_2p_3} \\ & + [b_7 + b_8\Delta_2^2 + b_9(\Delta_1^2 + \Delta_3^2) + b_{10}\Delta_2^2(\Delta_1^2 + \Delta_3^2) + b_{11}\Delta_1^2\Delta_3^2]\Delta_1\Delta_3 U^3_{p_1p_2p_3}, \end{aligned} \tag{21}$$

where

$$\begin{aligned} B_1 &= C_1/4 + 2(K_1 + K_2 + K_3)/a^2 & B_5 &= (-K_2/2 + K_4 + K_5)/a^2 \\ B_2 &= 2(K_1 + 2K_4)/a^2 & B_6 &= K_4/a^2 \\ B_3 &= C_1/4 + (K_1 - 2K_2)/a^2 & B_7 &= K_5/2a^2 \\ B_4 &= C_2/4 + K_2/a^2 & & \\ b_1 &= 2C_1 + 4C_2 + 16(K_1 + 2K_2 + K_3)/a^2 & b_7 &= 2C_1 + 8(K_1 + 2K_2 + 4K_4 + 2K_5)/a^2 \\ b_2 &= C_1 + 8(2K_1 + K_3 + 4K_7 + 2K_5)/a^2 & b_8 &= 16K_4/a^2 \\ b_3 &= C_2 + 4K_2/a^2 & b_9 &= 8(K_4 + K_5)/a^2 \\ b_4 &= C_1/2 + 4(K_1 + K_2 + K_3)/a^2 & b_{10} &= 4K_4/a^2 \\ b_5 &= 2(-K_2 + 2K_4 + 2K_5)/a^2 & b_{11} &= 4K_5/a^2 \\ b_6 &= 4(K_1 + 2K_4)/a^2 & & \end{aligned}$$

The corresponding equations for the equilibrium of the $\mathbf{e}_2$ and $\mathbf{e}_3$ components may be obtained by cyclical permutation.

For the particular boundary chosen, $p_1 = 0$ there are only two layers of particles, $p_1 = 0, 1$ on which there are boundary conditions. The boundary conditions on the normal $\mathbf{e}_1$ components are:

$$\begin{aligned}0 = {} & \alpha_1^i \overline{O}_0(\lambda_{110}^1 + \lambda_{101}^1) + \alpha_2^i \overline{O}_0(\lambda_{011}^1) + \alpha_3^i \overline{O}_0(\lambda_{002}^1 + \lambda_{020}^1) + \alpha_4^i [\overline{O}_3(\lambda_{110}^2) + \overline{O}_2(\lambda_{101}^3)] \\ & + \alpha_5^i [\overline{O}_3(\lambda_{011}^2) + \overline{O}_2(\lambda_{011}^3)] + \alpha_6^i [\overline{O}_3(\lambda_{020}^2) + \overline{O}_2(\lambda_{002}^3)] + \alpha_7^i \overline{O}_0(\lambda_{-110}^1 + \lambda_{-101}^1) \\ & + \alpha_8^i [\overline{O}_3(\lambda_{-110}^2) + \overline{O}_2(\lambda_{-101}^3)] + \alpha_9^i [\overline{O}_3(\lambda_{-121}^2) + \overline{O}_2(\lambda_{-112}^3)] + \alpha_{10}^i \overline{O}_0(\lambda_{-200}^1) \\ & + \alpha_{11}^i [\overline{O}_3(\lambda_{-211}^2) + \overline{O}_2(\lambda_{-211}^3)] + \alpha_{12}^i [\overline{O}_3(\lambda_{-220}^2) + \overline{O}_2(\lambda_{-202}^3)], \end{aligned} \tag{22}$$

and the boundary conditions on the tangential, $\mathbf{e}_2$ components are:

$$\begin{aligned}0 = {} & \beta_1^i \overline{O}_0(\lambda_{110}^2) + \beta_2^i \overline{O}_0(\lambda_{011}^2) + \beta_3^i \overline{O}_0(\lambda_{020}^2) + \beta_4^i \overline{O}_0(\lambda_{002}^2) + \beta_5^i \overline{O}_3(\lambda_{110}^1) \\ & + \beta_6^i \overline{O}_3(\lambda_{011}^1) + \beta_7^i \overline{O}_3(\lambda_{020}^1) + \beta_8^i \overline{O}_1(\lambda_{011}^3) + \beta_9^i \overline{O}_0(\lambda_{-110}^2) \\ & + \beta_{10}^i \overline{O}_0(\lambda_{-101}^2) + \beta_{11}^i \overline{O}_3(\lambda_{-110}^1) + \beta_{12}^i \overline{O}_3(\lambda_{-121}^1) + \beta_{13}^i \overline{O}_1(\lambda_{-121}^3 + \lambda_{-112}^3) \\ & + \beta_{14}^i \overline{O}_0(\lambda_{-200}^2) + \beta_{15}^i \overline{O}_3(\lambda_{-211}^1) + \beta_{16}^i \overline{O}_3(\lambda_{-220}^1), \end{aligned} \tag{23}$$

where the superscript i identifies the layer in which the particle is located, and the coefficients are:

$$\alpha_1^0 = \alpha_4^0 = \alpha_7^1 = -\beta_{11}^1 = K_3/2a^2, \qquad \alpha_2^0 = \beta_{10}^0 = 2(K_1 + 2K_4)/a^2,$$

$$\alpha_3^0 = \beta_{14}^0 = \beta_{14}^1 = (-K_2/2 + K_4 + K_5)/a^2, \qquad \alpha_5^0 = -\beta_6^0 = (3K_1 + K_4)/a^2,$$

$$\alpha_6^0 = -\beta_7^0 = (K_2 + K_3 + 2K_4 + K_5)/2a^2, \qquad \alpha_7^0 = \beta_9^0 = C_1/4 + 2(K_1 + K_2 + K_3)/a^2,$$

$$\alpha_8^0 = \beta_{11}^0 = -C_1/4 + (-K_1 + 2K_2)/a^2,$$

$$\alpha_9^0 = \alpha_{11}^0 = -\alpha_5^1 = \alpha_{11}^1 = -\beta_4^0 = \beta_{12}^0 = -\beta_{13}^0 = \beta_{15}^0 = \beta_6^1 = \beta_{15}^1 = -K_4/a^2,$$

$$\alpha_{10}^0 = \alpha_{10}^1 = C_2/4 + K_4/8a^2, \qquad \alpha_{12}^0 = -\alpha_6^1 = \alpha_{12}^1 = \beta_{16}^0 = \beta_7^1 = \beta_{16}^1 = -K_5/2a^2,$$

$$\alpha_1^1 = \alpha_4^1 = \alpha_9^1 = \beta_1^1 = \beta_2^1 = \beta_3^1 = \beta_4^1 = \beta_5^1 = \beta_8^1 = \beta_{10}^1 = \beta_{12}^1 = \beta_{13}^1 = 0,$$

$$\alpha_2^1 = 4K_4/a^2, \qquad \alpha_3^1 = K_5/a^2, \qquad \alpha_8^1 = \beta_1^0 = -\beta_5^0 = \beta_9^1 = (K_2 + K_3/2)/a^2$$

$$\beta_2^0 = 2K_1/a^2, \qquad \beta_3^0 = K_2/2a^2, \qquad \beta_8^0 = K_1/a^2$$

The boundary conditions on the tangential, $\mathbf{e}_3$ components may be obtained by a cyclical permutation on equation (23).

7. EVALUATION OF THE FORCE CONSTANTS

The seven force constants are determined in terms of the three classical elastic constants and the following frequencies, measured at the Brillouin zone boundaries:

1. ν_1, the frequency of a longitudinal wave in [100] direction;
2. ν_4, the frequency of a tangential wave in [100] direction;
3. ν_5, the frequency of a T_2 wave (wave vector parallel to $[1\bar{1}0]$) in [110] direction,
4. ν_7, the frequency of a tangential wave in [111] direction.

These conditions yield seven linearly independent equations for the seven force constants. The frequencies of the longitudinal waves at the Brillouin zone boundary in the

[110] and [111] directions, v_2 and v_3 respectively, and the frequency of the tangential, T_1, wave at the Brillouin zone boundary in the [110] direction, v_6, yield redundant expressions. The results for the force constants are:

$$\begin{aligned}
C_1 &= \{a[4C_{12}(3+4\sqrt{2})-4C_{44}(5+4\sqrt{2})-4C_{11}(1+2\sqrt{2})]+4\pi^2M[2v_4^2(4+3\sqrt{2}) \\
&\quad +v_1^2(1+\sqrt{2})+4v_7^2(3+2\sqrt{2})-16v_5^2]\}/16(1+\sqrt{2}), \\
C_2 &= \{a[4C_{11}(2+3\sqrt{2})+4C_{44}(5+4\sqrt{2})-4C_{12}(1+2\sqrt{2})-4\pi^2M[2v_4^2(4+3\sqrt{2}) \\
&\quad +v_1^2(1+\sqrt{2})+4v_7^2(3+2\sqrt{2})-16v_5^2]\}/16(1+\sqrt{2}), \\
K_1/a^2 &= \{a[4(C_{11}-C_{12}-C_{44})]+4\pi^2M[4v_7^2+2v_4^2(4+3\sqrt{2})-16v_5^2 \\
&\quad -v_1^2(1+\sqrt{2})]\}/64(1+\sqrt{2}), \\
K_2/a^2 &= \{a[2(1+2\sqrt{2})(C_{12}-C_{11})-2C_{44}(5+4\sqrt{2})]+4\pi^2M[2v_7^2(3+2\sqrt{2}) \\
&\quad +v_4^2(4+3\sqrt{2})-8v_5^2]\}/32(1+\sqrt{2}), \\
K_3/a^2 &= \{a[16\sqrt{2}C_{12}-16C_{44}-8C_{11}(1+3\sqrt{2})]+4\pi^2M[3v_1^2(1+\sqrt{2})+2v_4^2(7+3\sqrt{2}) \\
&\quad +8v_7^2(5+3\sqrt{2})-64v_5^2]\}/128(1+\sqrt{2}), \\
K_4/a^2 &= \{a[2(C_{12}+C_{44}-C_{11})]+4\pi^2M[8v_5^2-2v_7^2-v_4^2(3+2\sqrt{2})]\}/64(1+\sqrt{2}), \\
K_5/a^2 &= \{a[2\sqrt{2}(C_{12}-C_{11})-2C_{44}(2+\sqrt{2})]+4\pi^2M[2v_7^2(2+\sqrt{2})+v_4^2(3+2\sqrt{2}) \\
&\quad -8v_5^2]\}/32(1+\sqrt{2}). \qquad (24)
\end{aligned}$$

The sixth order terms in the finite difference equations of motion are contributed solely by the angular interactions represented by the force constants K_4 and K_5 [Figs. 1(f) and 1(g)]. If these interactions are eliminated, then the remaining interactions include those considered by Yuen and Varshni [5], represented by the force constants C_1, C_2, K_2, K_3, and an additional angular interaction represented by the force constant K_1. These five remaining force constants are determined in terms of the three classical elastic constants and the frequencies v_1 and v_4; the results are:

$$\begin{aligned}
C_1 &= [2a(C_{12}-C_{44})+\pi^2M(v_1^2+2v_4^2)]/4, \\
C_2 &= [a(C_{11}+2C_{44})-\pi^2M(v_1^2+2v_4^2)]/4, \\
K_1/a^2 &= \pi^2M(2v_4^2-v_1^2)/16, \\
K_2/a^2 &= [-aC_{44}+\pi^2Mv_4^2]/8, \\
K_3/a^2 &= [2a(3C_{44}-C_{12})+\pi^2M(3v_1^2-10v_4^2)]/32. \qquad (25)
\end{aligned}$$

If $v_1^2 = 2v_4^2$, then these become identical to Yuen and Varshni's results [5].

The sum of the distances between the three particles participating in an angular interaction is the least in the case of the interaction represented by the force constant K_1. If only this angular interaction, together with the two central force interactions, are considered, the force constants may be determined in terms of the three classical elastic constants as:

$$\begin{aligned} C_1 &= a(2C_{12}+C_{44})/3, \\ C_2 &= a(3C_{11}-2C_{12}-4C_{44})/12, \\ K_1/a^2 &= a(C_{44}-C_{12})/24. \end{aligned} \tag{26}$$

Svensson *et al.* [6] present the following data for copper at $T = 296°K$:

$$\begin{aligned} a &= 3{\cdot}147\times10^{-8}\text{ cm} & \nu_1 &= 7{\cdot}19\times10^{12}\text{ c/s} \\ C_{11} &= 16{\cdot}85\times10^{11}\text{ dyn/cm}^2 & \nu_4 &= 5{\cdot}08\times10^{12}\text{ c/s} \\ C_{12} &= 12{\cdot}15\times10^{11}\text{ dyn/cm}^2 & \nu_5 &= 4{\cdot}55\times10^{12}\text{ c/s} \\ C_{44} &= 7{\cdot}55\times10^{11}\text{ dyn/cm}^2 & \nu_7 &= 3{\cdot}37\times10^{12}\text{ c/s} \end{aligned}$$

Table 2 presents the resulting values of the force constants for the four models: the model containing seven interactions, the model containing five interactions, Yuen and Varshni's model with four interactions and the model with three interactions.

TABLE 2. THE FORCE CONSTANTS FOR COPPER AT $T = 296°K$. VALUES IN UNITS OF 10^3 dyn/cm

Force constant	Seven interaction model	Five interaction model	Yuen and Varshni model	Three interaction model
C_1	37·26	35·20	35·22	38·38
C_2	−0·0751	1·984	1·962	−1·189
K_1/a^2	0·1324	−0·00542		−0·6953
K_2/a^2	0·4616	−0·05297	−0·0476	
K_3/a^2	−0·0697	−0·9871	−0·9917	
K_4/a^2	−0·0689			
K_5/a^2	0·3262			

The dispersion curves for longitudinal and transverse bodily waves in the [100], [110] and [111] directions were computed for each model and are compared to the experimental results in Figs. 2(a)–(c). The results obtained from the model containing only three interactions, two central force and one angular (K_1), are clearly inferior to those obtained by Yuen and Varshni. The model containing five interactions (Yuen and Varshni's model plus K_1) yields results which are indistinguishable from those of Yuen and Varshni. The model containing seven interactions yields results which show a small, but significant, improvement in the match with the experimental results.

8. SHEAR WAVES

In an infinite lattice, $-\infty < p_1, p_2, p_3 < \infty$, consider displacements

$$\begin{aligned} U^1_{p_1p_2p_3} &= U^3_{p_1p_2p_3} = 0, \\ U^2_{p_1p_2p_3} &= f(p_1)e^{i(p_3\theta-\omega t)}. \end{aligned} \tag{27}$$

These displacements represent waves with displacement perpendicular to the wave-normal and parallel to the principal crystallographic plane $p_1 = \text{const}$. With these displacements, the first and third equations of the type (21) are satisfied identically and the second is satisfied if

$$0 = b_5\Delta_1^4 f(p_1)+[b_2-2b_6(1-\cos\theta)]\Delta_1^2 f(p_1)+[-2b_2(1-\cos\theta) +4b_5(1-\cos\theta)^2+M\omega^2]f(p_1)$$

Assuming solutions of the form $f(p_1) = A\,e^{\xi p_1}$ yields:

$$(1-\cos\xi_{1,2}) = \{[b_2-2b_6(1-\cos\theta)]\pm[b_2^2-4b_5M\omega^2+4b_2(2b_5-b_6)(1-\cos\theta) +4(b_6^2-4b_5^2)(1-\cos\theta)^2]^{\frac{1}{2}}\}/4b_5. \tag{28}$$

The general solution for the displacements is then:

$$U^2_{p_1p_2p_3} = [A_1\cos\xi_1p_1+A_2\cos\xi_2p_2]\,e^{i(p_3\theta-\omega t)}+[A_3\sin\xi_1p_1+A_4\sin\xi_2p_2]e^{i(p_3\theta-\omega t)}, \tag{29}$$

where the $\xi_{1,2}$ are, in general, complex numbers. As may be seen from equation (29) the solution is separable into two parts: one symmetric, and one antisymmetric about the plane $p_1 = 0$.

The behavior of the roots $\xi_{1,2}$ of equation (28), as functions of the frequency, will now be analyzed. Let

$$1-\cos\xi_{1,2} = \phi_{1,2}, \qquad \xi_{1,2} = \chi_{1,2}+i\psi_{1,2}$$

then

$$\cos\xi_j = \cos\chi_j\cosh\psi_j - i\sin\chi_j\sinh\psi_j = 1-\phi_j, \qquad j = 1,2.$$

For

$$\omega^2 \le \omega_c^2 = [b_2^2+4b_2(2b_5-b_6)(1-\cos\theta)+4(b_6^2-4b_5^2)(1-\cos\theta)^2]/4b_5M,$$

the parameters ϕ_j are real. In this case

$$\sin\chi_j\sinh\psi_j = 0$$

and there are three regions:

1. $\phi_j < 0$: the roots are $\xi_j = i\psi_j$ where $\cosh\psi_j = 1-\phi_j$;
2. $0 \le \phi_j \le 2$: the roots are $\xi_j = \chi_j$ where $\cos\chi_j = 1-\phi_j$;
3. $\phi_j > 2$: the roots are $\xi_j = \pi+i\psi_j$ where $\cosh\psi_j = \phi_j-1$;

Now, the minimum value of ϕ_1 occurs when $\omega = \omega_c$. This minimum value is:

$$\phi_{1\min} = [b_2-2b_6(1-\cos\theta)]/4b_5,$$

which for most materials, is $\gg 2$, since it is essentially a ratio of the lowest to a higher order interaction. Consequently, the first root is $\xi_1 = \pi+i\psi_1$, where $\cosh\psi_1 = \phi_1-1$.

For the second root, define:

$$\omega_a^2 = 2(1-\cos\theta)[b_2-2b_5(1-\cos\theta)]/M,$$

$$\omega_b^2 = \{2(1-\cos\theta)[b_2-2b_5(1-\cos\theta)]+4[b_2-4b_5-2b_6(1-\cos\theta)]\}/M,$$

then: for $0 \leq \omega < \omega_a$, then $\phi_2 < 0$, and the second root is $\xi_2 = i\psi_2$, where $\cosh \psi_2 = 1 - \phi_2$; for $\omega_a \leq \omega \leq \omega_b$, then $0 \leq \phi_2 \leq 2$, and the second root is $\xi_2 = \chi_2$, where $\cos \chi_2 = 1 - \phi_2$; for $\omega_b < \omega \leq \omega_c$, then $\phi_2 > 2$, and the second root is $\xi_2 = \pi + i\psi_2$, where $\cosh \psi_2 = \phi_2 - 1$.

For high frequencies, $\omega > \omega_c$, the parameters $\phi_{1,2}$ are complex conjugates. For this case, define:

$$\phi_{1,2} = \alpha_1 \pm i\alpha_2$$

then

$$1 - \alpha_1 \pm i\alpha_2 = \cos \chi_{1,2} \cosh \psi_{1,2} - i \sin \chi_{1,2} \sinh \psi_{1,2}.$$

Substituting $\chi_{1,2} = \pi \pm \bar{\chi}$ and simplifying yields $\xi_{1,2} = \pi \pm \bar{\chi} + i\psi$, where $\psi_1 = \psi_2 = \psi$.

The graphs of $\xi_j = \xi_j(\omega^2)$ are given in Fig. 3. For $\omega < \omega_c$ the graph of $\xi_1 = \xi_1(\omega^2) = \pi + i\psi_1$ is a smooth curve, rising vertically at $\omega = 0$, thereafter with continuously decreasing slope until at $\omega = \omega_c$ the curve becomes horizontal. For $\omega < \omega_c$, the graph of $\xi_2 = \xi_2(\omega^2)$

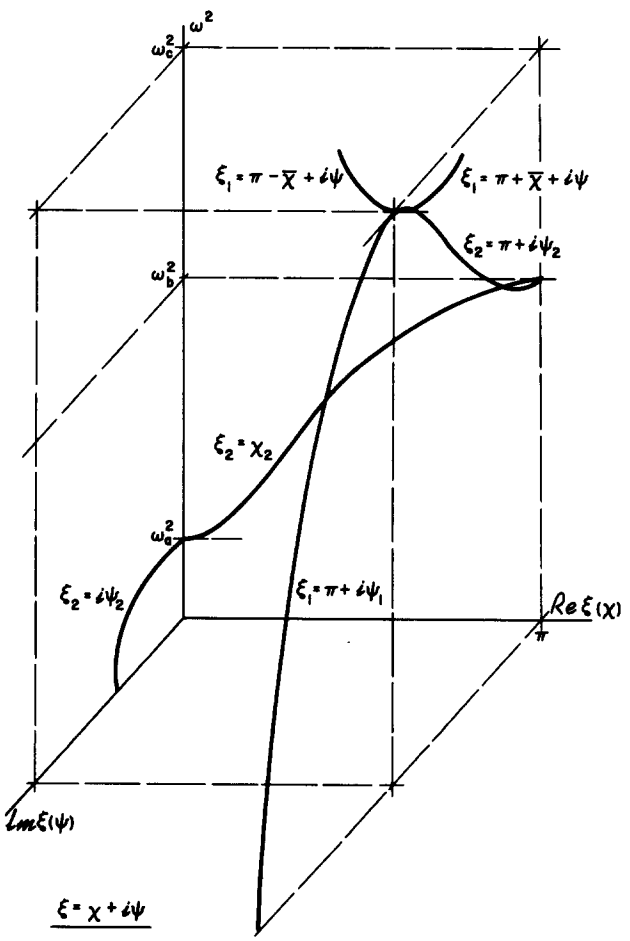

FIG. 3. Graph of the roots $\xi_j = \xi_j(\omega^2)$, $j = 1, 2$.

is composed of three smooth curves: the first curve, $\xi_2 = i\psi_2$, rises vertically at $\omega = 0$, thereafter with continuously decreasing slope until at $\omega = \omega_a$, $\xi_2 = 0$, and the curve becomes horizontal; the second curve, $\xi_2 = \chi_2$ starts horizontally at $\omega = \omega_a$, $\xi_2 = 0$ and rises until it again becomes horizontal at $\omega = \omega_b$, $\xi_2 = \pi$; the third curve, $\xi_2 = \pi + i\psi_2$ starts horizontally at $\omega = \omega_b$, $\xi_2 = \pi$ and rises until it again becomes horizontal at $\omega = \omega_c$. For $\omega > \omega_c$ the graphs of $\xi_{1,2} = \xi_{1,2}(\omega^2) = \pi \pm \bar{\chi} + i\psi$ are two smooth curves, each the image of the other reflected in the $\xi = \pi$ plane.

9. THICKNESS–TWIST WAVES IN A COPPER PLATE

Consider an infinite plate bounded by the free surfaces $p_1 = \pm N$. The waves described in the previous section, propagating along this plate, are called thickness–twist waves. Substituting the solution of that section, equation (29) into the difference operator $\bar{O}_\alpha(\lambda^\beta_{h_1h_2h_3})$ defined in Section 3(a), results in:

$$\bar{O}_0(\lambda^2_{h_1h_2h_3}) = 4[A_1 g_{11}(h_1, h_3, p_1) + A_2 g_{12}(h_1, h_3, p_1) + A_3 g_{21}(h_1, h_3, p_1) + A_4 g_{22}(h_1, h_3, p_1)]e^{i(p_1\theta - \omega t)},$$

where

$$g_{1j}(h_1, h_3, p_1) = \cos(h_3\theta)\cos\xi_j(h_1 + p_1) - \cos\xi_j p_1,$$
$$g_{2j}(h_1, h_3, p_1) = \cos(h_3\theta)\sin\xi_j(h_1 + p_1) - \sin\xi_j p_1, \qquad j = 1, 2.$$

Consider, first, only the symmetric solution. The boundary conditions yield; for $p_1 = -N$

$$\begin{aligned} 0 = {} & A_1[\beta^0_1 g_{11}(1, 0, -N) + \beta^0_2 g_{11}(0, 1, -N) + \beta^0_4 g_{11}(0, 2, -N) + \beta^0_9 g_{11}(-1, 0, -N) \\ & + \beta^0_{10} g_{11}(-1, 1, -N) + \beta^0_{14} g_{11}(-2, 0, -N)] + A_2[\beta^0_1 g_{12}(1, 0, -N) + \beta^0_2 g_{12}(0, 1, -N) \\ & + \beta^0_4 g_{12}(0, 2, -N) + \beta^0_9 g_{12}(-1, 0, -N) + \beta^0_{10} g_{12}(-1, 1, -N) + \beta^0_{14} g_{12}(-2, 0, -N)] \end{aligned} \tag{30}$$

and, for $p_1 = -N + 1$

$$\begin{aligned} 0 = {} & A_1[\beta^1_9 g_{11}(-1, 0, -N+1) + \beta^1_{14} g_{11}(-2, 0, -N+1)] \\ & + A_2[\beta^1_9 g_{12}(-1, 0, -N+1) + \beta^1_{14} g_{12}(-2, 0, -N+1)]. \end{aligned} \tag{31}$$

Now,

$$g_{1j}(h_1, h_3, p_1) = g_{1j}(-h_1, h_3, -p_1), \quad \text{and} \quad g_{2j}(h_1, h_3, p_1) = -g_{2j}(-h_1, h_3, -p_1),$$

so the boundary conditions at $p_1 = N, N-1$ yield no additional information.

Setting the determinant of the coefficients in the boundary conditions equal to zero yields the secular equations:

$$\begin{aligned} 0 = {} & [\beta^1_9 P_1]\cos\xi_1 N \cos\xi_2 N + [\beta^1_9 P_2 + 2\beta^1_{14} P_5]\cos\xi_1 N \sin\xi_2 N \sin\xi_2 \\ & + [\beta^1_9 P_3 + 2\beta^1_{14} P_6]\sin\xi_1 N \cos\xi_2 N \sin\xi_1 + [(\beta^1_9 + 2\beta^1_{14})P_4]\sin\xi_1 N \sin\xi_2 N, \end{aligned} \tag{32a}$$

for the symmetric case and

$$0 = [\beta_9^1 P_1] \sin \xi_1 N \sin \xi_2 N - [\beta_9^1 P_2 + 2\beta_{14}^1 P_5] \sin \xi_1 N \cos \xi_2 N \sin \xi_2$$
$$- [\beta_9^1 P_3 + 2\beta_{14}^1 P_6] \cos \xi_1 N \sin \xi_2 N \sin \xi_1 + [(\beta_9^1 + 2\beta_{14}^1) P_4] \cos \xi_1 N \cos \xi_2 N, \quad (32b)$$

for the antisymmetric case, where

$$P_1 = [M_1 + 2M_2\phi_1\phi_2](\phi_1 - \phi_2), \qquad P_4 = -2M_2(\phi_1 - \phi_2) \sin \xi_1 \sin \xi_2,$$
$$P_2 = M_1 + 2M_3\phi_1 + 2M_2\phi_1[3 - (\phi_1 + \phi_2)], \qquad P_5 = M_1 + M_4\phi_1 + 2M_2\phi_1(2 - \phi_1),$$
$$P_3 = -\{M_1 + 2M_3\phi_2 + 2M_2\phi_2[3 - (\phi_1 + \phi_2)]\}, \qquad P_6 = -\{M_1 + M_4\phi_2 + 2M_2\phi_2(2 - \phi_2)\},$$

and

$$M_1 = (\beta_2^0 + \beta_{10}^0)(1 - \cos\theta) + \beta_4^0(1 - \cos 2\theta), \qquad M_3 = \beta_9^0 + \beta_{10}^0 \cos\theta,$$
$$M_2 = \beta_{14}^0, \qquad M_4 = \beta_1^0 + \beta_9^0 + \beta_{10}^0 \cos\theta.$$

In Section 8 it was shown that for most materials, $\phi_1 \geq [b_2 - 2b_6(1 - \cos\theta)]/4b_5 \gg 2$. Then $\xi_1 = \pi + i\psi_1$, where $\cosh \psi_1 = \phi_1 - 1 \gg 2$, and therefore

$$\cos \xi_1 N = \cos(\pi + i\psi_1)N = (-1)^N \cosh \psi_1 N$$
$$\sin \xi_1 N = \sin(\pi + i\psi_1)N = (-1)^N \sinh \psi_1 N$$

Now, unless N is very small, the argument of the hyperbolic functions, $\psi_1 N$ is quite large and the approximation $\cosh \psi_1 N \approx \sinh \psi_1 N$ is valid. Using this approximation, the secular equations may be reduced to

$$0 = \{\beta_9^1 P_1 + i[\beta_9^1 P_3 + 2\beta_{14}^1 P_6] \sin \xi_1\} \cos \xi_2 N$$
$$+ \{[\beta_9^1 P_2 + 2\beta_{14}^1 P_5] \sin \xi_2 + i[(\beta_9^1 + 2\beta_{14}^1) P_4]\} \sin \xi_2 N, \quad (33a)$$

for the symmetric case and

$$0 = \{[\beta_9^1 P_2 + 2\beta_{14}^1 P_5] \sin \xi_2 + i[(\beta_9^1 + 2\beta_{14}^1) P_4]\} \cos \xi_2 N$$
$$- \{\beta_9^1 P_1 + i[\beta_9^1 P_3 + 2\beta_{14}^1 P_6] \sin \xi_1\} \sin \xi_2 N, \quad (33b)$$

for the antisymmetric case. These are the secular equations employed in the present calculations.

Figure 4 presents the real branches of the dispersion relation for the thickness-twist waves in a plate 15 layers thick: $N = 7$. The parameter s identifying each curve is the number of nodes through the thickness; the curves with an even number of nodes are the symmetric solutions, those with an odd number are the antisymmetric solutions.

Analysis of the problem by the theory of elasticity leads to the well known dispersion relation which may be written as:

$$\omega_{\text{cont}} = (\pi/2h)\sqrt{C_{44}/\rho}[s^2 + (2h\eta/\pi)^2]^{\frac{1}{2}},$$
$$= [2\pi/(2N+1)a]\sqrt{[C_{44}/\rho]}[s^2 + (4h\theta/\pi a)]^{\frac{1}{2}}, s = 0, 1, 2, \ldots. \quad (34)$$

where $2h = (2N+1)(a/2)$ is the plate thickness and $\eta = 2\theta/a$ is the wave number. The cutoff frequency for the first antisymmetric mode, i.e. $\omega_{\text{cont}}(s = 1, \eta = 0)$, is denoted as $\bar{\omega}$

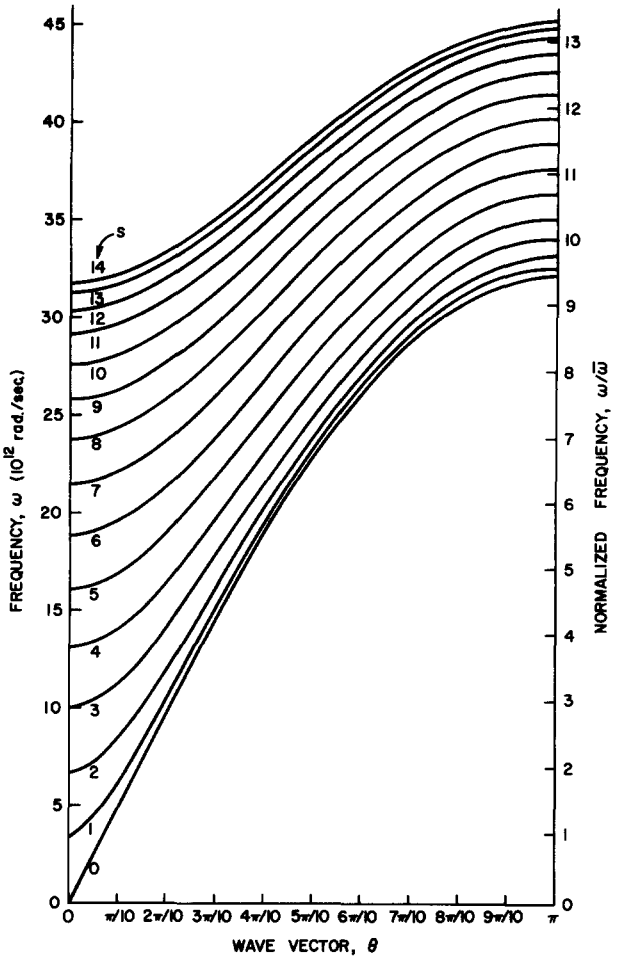

FIG. 4. The real branches of the dispersion relation for $N = 7$: face-shear ($S = 0$) and thickness-twist ($S = 1, \ldots 14$) waves in a plate.

and is used as a reference frequency. This reference frequency has the value $3{\cdot}38 \times 10^{12}$ rad./sec in the present case. The normalized frequencies for the continuum are then:

$$\omega_{\text{cont}}/\bar{\omega} = [s^2 + (2h\eta/\pi)^2]^{\frac{1}{2}} = [s^2 + (4h\theta/\pi a)^2]^{\frac{1}{2}}, \qquad s = 0, 1, 2, \ldots. \tag{35}$$

The infinity of real branches of this continuum dispersion relation are all hyperbolic curves extending from low frequency cutoffs at $\eta = 0$, $\omega_{\text{cont}}/\bar{\omega} = 0, 1, 2, \ldots, \infty$ to infinite frequencies and wave numbers. On the other hand there are only a finite number, $2N+1$, of modes of vibration for the lattice, corresponding to $0, 1, 2, \ldots, 2N$ nodes through the plate thickness, and therefore only $2N+1$ branches in the dispersion relation. Each of these branches has a high frequency cutoff at $\theta = \pi$ in addition to a low frequency cutoff*

* For the present case, these low frequency cutoffs are very closely approximated by:

$$\omega/\bar{\omega} = \left[\frac{\partial(\partial N+1)}{\pi}\sin\frac{\pi s}{2(2N+1)}\right] - 0{\cdot}00122\left[\frac{\partial(\partial N+1)}{\pi}\sin\frac{\pi s}{2(2N+1)}\right]^2, s = 0, 1, \ldots < 2N+1$$

at $\theta = 0$. Therefore the continuum is a good approximation to the lattice only in the low frequency, long wavelength ($\lambda = \pi a/\theta$) region. All wavelengths, along and through the thickness of the plate, must be large in comparison to a for the continuum approximation to be valid.

The displacements are given by:

$$U^2_{p_1p_2p_3} = A_2[(A_1/A_2)(-1)^{p_1}\cosh\psi_1 p_1 + \cos\xi_2 p_1]e^{i(p_3\theta-\omega t)}, \tag{36a}$$

for the symmetric case and

$$U^2_{p_1p_2p_3} = A_4[(A_3/A_4)(-1)^{p_1}\sinh\psi_1 p_1 + \sin\xi_2 p_1]e^{i(p_3\theta-\omega t)}, \tag{36b}$$

for the antisymmetric case, where, from the $p_1 = -N+1$ boundary condition

$$A_1/A_2 = \frac{(-1)^{N+1}\{[\beta^1_9\phi_2]\cos\xi_2 N - [(\beta^1_9+2\beta^1_{14})\sin\xi_2]\sin\xi_2 N\}}{\cosh\psi_1 N[\beta^1_9\phi_1 - (\beta^1_9+2\beta^1_{14})(\phi_1^2-2\phi_1)^{\frac{1}{2}}]},$$

$$A_3/A_4 = \frac{(-1)^{N+1}\{[\beta^1_9\phi_2]\sin\xi_2 N + [(\beta^1_9+2\beta^1_{14})\sin\xi_2]\cos\xi_2 N\}}{\cosh\psi_1 N[\beta^1_9\phi_1 - (\beta^1_9+2\beta^1_{14})(\phi_1^2-2\phi_1)^{\frac{1}{2}}]}.$$

The mode shapes for $\theta = 0$ are shown in Fig. 5. It is apparent that for the first few modes the mode shapes are close approximations to sinusoidal curves, and it is for these modes that the continuum approximation is valid. However as the number of nodes through the thickness increases, the mode shapes differ more and more markedly from sinusoidal curves and the continuum approximation loses its validity even for long wavelengths along the plate.

The displacements consist of the sum of two waves across the thickness of the plate. The first wave has a complex wave number, $\xi_1 = \pi + i\psi_1$, the second, a real wave number, $\xi_2 = \chi_2$. The variation of these wave numbers with the wave number along the plate, θ, for $0 \leq \theta \leq \pi$, is slight: ψ_1 remains constant to within 0·1 per cent, while χ_2 varies by about 3 per cent. Therefore the mode shapes remain essentially constant as the wavelength along the plate varies.

Mindlin [3] has analyzed the problem of the thickness–twist vibrations for a lattice plate consisting of a simple cubic material having nearest and next-nearest neighbor central force interactions and angular interactions between three successive, non-collinear particles. He obtains the following closed form solutions for the dispersion relations and the displacements

$$\omega/\bar{\omega} = [2(2N+1)/\pi]\left[\sin^2\frac{\pi s}{2(2N+1)} + \sin^2(\theta/2)\right],$$

$$U^2_{p_1p_2p3} = \left[A_1\cos\frac{\pi s p_1}{2N+1} + A_2\sin\frac{\pi s p_1}{2N+1}\right]e^{i(p_3\theta-\omega t)}, \qquad s = 0, 1, \ldots < 2N+1.$$

The displacements here are given by one wave across the thickness with wave number $s\pi/(2N+1)$. If $\bar{\omega}$ is assigned the value $3{\cdot}38\times10^{12}$ rad./sec, its value for the present case, these equations give results for the dispersion curves and mode shapes which are indistinguishable from those presented in Figs. 4 and 5.

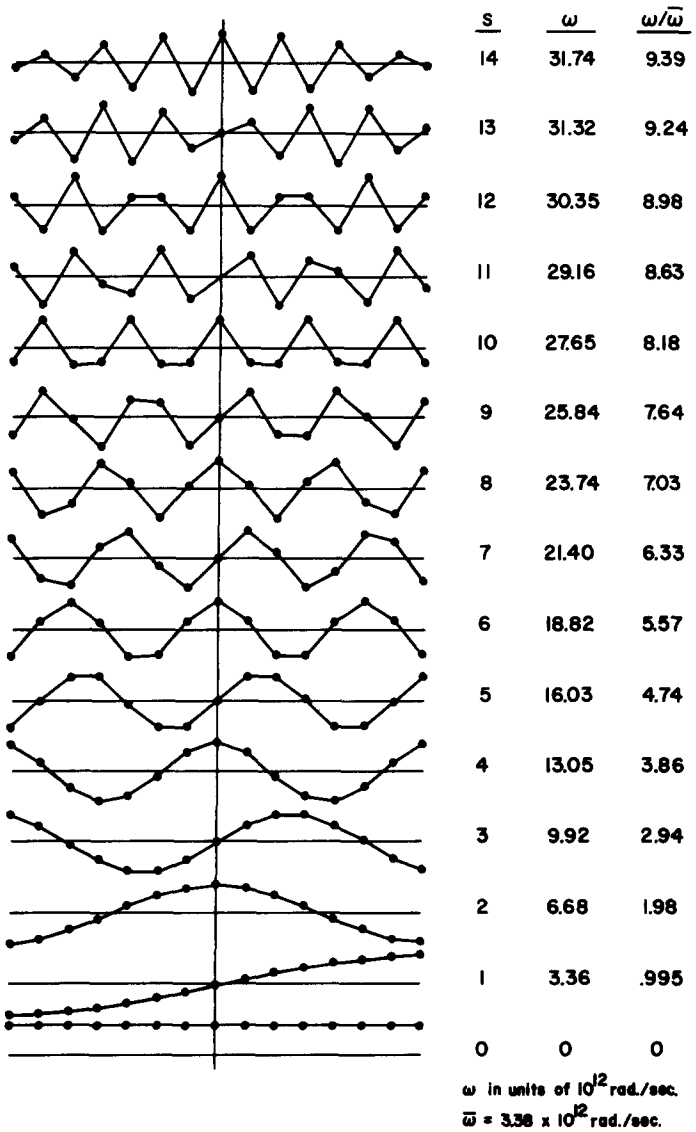

FIG. 5. Frequencies and mode shapes, $\theta = 0$.

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APPENDIX

The difference operators may be written as:

$$O_0(\lambda^\alpha_{h_1h_2h_3}) = [(E_1^{h_1}+\bar{E}_1^{h_1})(E_2^{h_2}+\bar{E}_2^{h_2})(E_3^{h_3}+\bar{E}_3^{h_3})-8I]U^\alpha_{p_1p_2p_3},$$

$$O_1(\lambda^\alpha_{h_1h_2h_3}) = [(E_1^{h_1}+\bar{E}_1^{h_1})(E_2^{h_2}-\bar{E}_2^{h_2})(E_3^{h_3}-\bar{E}_3^{h_3})]U^\alpha_{p_1p_2p_3},$$

$$O_2(\lambda^\alpha_{h_1h_2h_3}) = [(E_1^{h_1}-\bar{E}_1^{h_1})(E_2^{h_2}+\bar{E}_2^{h_2})(E_3^{h_3}-\bar{E}_3^{h_3})]U^\alpha_{p_1p_2p_3},$$

$$O_3(\lambda^\alpha_{h_1h_2h_3}) = [(E_1^{h_1}-\bar{E}_1^{h_1})(E_2^{h_2}-\bar{E}_2^{h_2})(E_3^{h_3}+\bar{E}_3^{h_3})]U^\alpha_{p_1p_2p_3}.$$

Then, expanding the terms:

$$E_1^{h_1}+\bar{E}_1^{h_1} = (1+\Delta_1^+)^{h_1}+(1-\Delta_1^-)^{h_1}$$

$$= 2+h_1(\Delta_1^+-\Delta_1^-)+\frac{h_1(h_1-1)}{2!}(\Delta_1^{+2}+\Delta_1^{-2})+\frac{h_1(h_1-1)(h_1-2)}{3!}(\Delta_1^{+3}-\Delta_1^{-3})$$

$$+\frac{h_1(h_1-1)(h_1-2)(h_1-3)}{4!}(\Delta_1^{+4}+\Delta_1^{-4})+\ldots,$$

$$E_1^{h_1}-\bar{E}_1^{h_1} = (1+\Delta_1^+)^{h_1}-(1-\Delta_1^-)^{h_1}$$

$$= h_1(\Delta_1^++\Delta_1^-)+\frac{h_1(h_1-1)}{2!}(\Delta_1^{+2}-\Delta_1^{-2})+\frac{h_1(h_1-1)(h_1-2)}{3!}(\Delta_1^{+3}+\Delta_1^{-3})$$

$$+\frac{h_1(h_1-1)(h_1-2)(h_1-3)}{4!}(\Delta_1^{+4}-\Delta_1^{-4})+\cdots.$$

And, in terms of the central differences:

$$\Delta_\alpha^+-\Delta_\alpha^- = \Delta_\alpha^2,\ \Delta_\alpha^++\Delta_\alpha^- = 2\Delta_\alpha,\ \Delta_\alpha^{+2}+\Delta_\alpha^{-2} = \Delta_\alpha^4+2\Delta_\alpha^2,\ \Delta_\alpha^{+2}-\Delta_\alpha^{-2} = 2\Delta_\alpha^2\Delta_\alpha,$$

$$\Delta_\alpha^{+3}-\Delta_\alpha^{-3} = \Delta_\alpha^6+2\Delta_\alpha^4,\ \Delta_\alpha^{+3}+\Delta_\alpha^{-3} = 2\Delta(\Delta_\alpha^4+\Delta_\alpha^2),\ \Delta_\alpha^{+4}+\Delta_\alpha^{-4} = \Delta_\alpha^8+4\Delta_\alpha^6+3\Delta_\alpha^4,$$

$$\Delta_\alpha^{+4}-\Delta_\alpha^{-4} = 2\Delta_\alpha(\Delta_\alpha^6+2\Delta_\alpha^4),\ldots.$$

Then

$$E_1^{h_1}+\bar{E}_1^{h_1} = 2+h_1^2\Delta_1^2+\frac{h_1(h_1-1)}{2!}(\Delta_1^4+2\Delta_1^2)+\frac{h_1(h_1-1)(h_1-2)}{3!}(\Delta_1^6+3\Delta_1^4)$$

$$+\frac{h_1(h_1-1)(h_1-2)(h_1-3)}{4!}(\Delta_1^8+4\Delta_1^6+2\Delta_1^4)+\ldots,$$

$$E_1^{h_1}-\bar{E}_1^{h_1} = 2h_1\Delta_1+\frac{h_1(h_1-1)}{2!}2\Delta_1^2\Delta_1+\frac{h_1(h_1-1)(h_1-2)}{3!}(\Delta_1^4+\Delta_1^2)2\Delta_1$$

$$+\frac{h_1(h_1-1)(h_1-2)(h_1-3)}{4!}(\Delta_1^6+2\Delta_1^4)2\Delta_1+\ldots.$$

The final forms are obtained by substituting these terms into the expressions for the operators.

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Абстракт—Определяются конечно разностные уравнения движения шестого порядка и присоединенные краевые условия для главных плоскостей для гранецентрированной кубической сетки массовых частиц. Решаются уравнения для волн сдвигов грани и сдвигов по толщине, в пластинке с двумя свободными гранями. Дается расчет видов колебаний и спектры частоты для меди. Результаты сравниваются с предыдущим решением для простого кубического материала и с решением классических уравнений упругости.