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Research and Development Report

TRIO, A COMPUTER PROGRAM FOR THE
CALCULATION OF PHONON DISPERSION CURVES,
ATOM POLARIZATION VECTORS, AND NORMALIZED
STRUCTURE FACTORS

by

Thomas Stephen Prevender

October 1969

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TRIO, A COMPUTER PROGRAM FOR THE CALCULATION OF PHONON DISPERSION
CURVES, ATOM POLARIZATION VECTORS, AND NORMALIZED STRUCTURE FACTORS

Thomas Stephen Prevender[†]

ABSTRACT

A computer program is described that calculates the phonon dispersion curves, atom polarization vectors, and normalized inelastic neutron scattering structure factors for materials possessing the CsCl structure. The input data for the program include a set of Born von Karman-type force constants. The program is written in FORTRAN for use with an IBM 360-65 computer.

[†]Present address: Sandia Laboratories, P. O. Box 5800,
Albuquerque, New Mexico 87115.

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1. INTRODUCTION

In the harmonic approximation of lattice dynamics¹ the potential energy of a crystal is expressed as a Taylor's series in powers of the atomic displacements where only terms to second order are retained. The α -th Cartesian component of the displacement of the s -th atom in the ℓ -th unit cell will be denoted by $u_\alpha(\ell, s)$. The potential energy of the solid may then be written as

$$\begin{aligned} \Phi = & \Phi_0 + \sum_{\ell, s, \alpha} \left. \frac{\partial \Phi}{\partial U_\alpha(\ell, s)} \right|_0 U_\alpha(\ell, s) \\ & + \frac{1}{2} \sum_{\substack{\ell, s, \alpha \\ \ell', s', \beta}} \left. \frac{\partial^2 \Phi}{\partial U_\alpha(\ell, s) \partial U_\beta(\ell', s')} \right|_0 U_\alpha(\ell, s) U_\beta(\ell', s'). \end{aligned} \quad (1)$$

In Eq. (1) the subscript zero signifies that the coefficients in the expansion are evaluated in the equilibrium configuration. Since the linear terms vanish at equilibrium, Eq. (1) may be rewritten as

$$\Phi = \Phi_0 + \frac{1}{2} \sum_{\substack{\ell, s, \alpha \\ \ell', s', \beta}} \phi_{\alpha\beta}(\ell\ell', ss') U_\alpha(\ell, s) U_\beta(\ell', s'), \quad (2)$$

where

$$\phi_{\alpha\beta}(\ell\ell', ss') = \left. \frac{\partial^2 \Phi}{\partial U_\alpha(\ell, s) \partial U_\beta(\ell', s')} \right|_0. \quad (3)$$

The equation of motion of the (ℓ, s) atom is

$$M_s \ddot{U}_\alpha(\ell, s) = - \frac{\partial \Phi}{\partial U_\alpha(\ell, s)} = - \sum_{\ell', s', \beta} \phi_{\alpha\beta}(\ell\ell', ss') U_\beta(\ell', s'). \quad (4)$$

Equation (4) represents a set of 3SN simultaneous equations where S is the number of atoms per unit cell and N is the number of unit cells in the solid. These equations may be simplified by the assumption that the displacements may be represented as a superposition of traveling waves, i.e.,

$$U_{\alpha}(\ell, s) = \sum_{\bar{q}, j} \left[\frac{1}{\sqrt{M_s}} \right] (\bar{q}, j) \frac{\bar{e}_s(\bar{q}, j)}{\sqrt{M_s}} e^{i\bar{q} \cdot [\bar{\ell} + \bar{s}]} e^{-i\omega\tau}. \quad (5)$$

Here, $\underline{q}$ and j are the wave vector and polarization index respectively of the traveling wave (phonon). The polarization vector of the s -th atom is $\underline{e}_s(\underline{q}, j)$, and $U(\underline{q}, j)$ may be thought of as the amplitude associated with the wave. If Eqs. (4) and (5) are combined, the result is

$$e_{\alpha s}(\bar{q}, j) \omega^2 j(\bar{q}) = \sum_{\ell', \bar{s}', \beta} (M_s M_{s'})^{-1/2} \phi_{\alpha\beta}(\ell\ell', ss') e^{i\bar{q} \cdot [(\bar{\ell}' - \bar{\ell}) + (\bar{s}' - \bar{s})]} e_{\beta s'}(\bar{q}, j). \quad (6)$$

The dynamical matrix D is defined such that the $\alpha\beta$ -th element is

$$D_{\alpha\beta}^{ss'} = \sum_{\ell'} (M_s M_{s'})^{-1/2} \phi_{\alpha\beta}(\ell\ell', ss') e^{i\bar{q} \cdot [(\bar{\ell}' - \bar{\ell}) + (\bar{s}' - \bar{s})]}. \quad (7)$$

With this definition, Eq. (6) may be written as

$$\sum_{s', \beta} (D_{\alpha\beta}^{ss'}(\bar{q}) - \omega^2 j(\bar{q}) \delta_{ss'} \delta_{\alpha\beta}) e_{\beta s'} = 0. \quad (8)$$

The condition that the set of equations denoted by Eq. (8) has a solution is that the determinant of the coefficient be zero, i.e.,

$$\det | D_{\alpha\beta}^{ss'}(\bar{q}) - \omega^2 j(\bar{q}) \delta_{ss'} \delta_{\alpha\beta} | = 0. \quad (9)$$

Equations (9) and (8) may be solved to obtain the dispersion relations, $v_j(q)$, and the atomic polarization vectors $\underline{e}_s$.

2. DESCRIPTION OF PROGRAM

A. Dispersion curves

TRIO calculates the dispersion curves for q , in a specified direction by solving Eq. (9). The components of the dynamical matrix ($D_{\alpha\beta}^{ss'}(q)$) have previously been obtained for models that include fourth² and sixth³ neighbor interactions. The force constants ($\phi_{\alpha\beta}(\ell\ell',ss')$) that must be supplied as input data may be obtained from the phonon dispersion curves through the use of least-squares fitting programs.⁴

B. Polarization vectors

TRIO finds the atom polarization vectors for q in a specified direction by solving Eqs. (8) and (9). The polarization vectors have been chosen to obey the orthonormality and closure relations

$$\sum_{s,\alpha} e_{s\alpha}^*(\bar{q},j) e_{s\alpha}(\bar{q},j') = \delta_{jj'} \quad (10)$$

and

$$\sum_j e_{s\alpha}(\bar{q},j) e_{s'\beta}^*(\bar{q},j) = \delta_{\alpha\beta} \delta_{ss'} \quad (11)$$

C. Normalized structure factor

The differential scattering cross-section⁵ for one-phonon coherent neutron scattering processes is proportional to the inelastic structure factor, $|F_j|^2$, where

$$|F_j|^2 = \left| \sum_s (M_s)^{-1/2} b_s \bar{Q} \cdot \bar{e}_s(\bar{q}, j) e^{i\bar{\tau} \cdot \bar{R}_s} e^{-W_s} \right|^2. \quad (12)$$

Here $\bar{Q}$ is the scattering vector, $\bar{\tau}$ is the reciprocal lattice vector nearest to $\bar{Q}$ and the W_s are the Debye-Waller factors. For the case of the CsCl lattice, $s = 0$ refers to the origin atom and $s = 1$ refers to the atom at $(1\ 1\ 1)^a/2$. The coherent scattering length⁶ of the atom at $\bar{R}_s$ is b_s .

If Eq. (12) is expanded it becomes

$$\begin{aligned} |F_j|^2 = & \frac{[\bar{Q} \cdot \bar{e}_0(\bar{q}, j)]^2 b_0^2}{M_0} e^{-2W_0} \\ & + \frac{2[\bar{Q} \cdot \bar{e}_0(\bar{q}, j)][\bar{Q} \cdot \bar{e}_1(\bar{q}, j)] b_0 b_1}{\sqrt{M_0 M_1}} \cos \pi(T_1 + T_2 + T_3) e^{-(W_0 + W_1)} \\ & + \frac{[\bar{Q} \cdot \bar{e}_1(\bar{q}, j)]^2}{M_1} b_1^2 e^{-2W_1}. \end{aligned} \quad (13)$$

As illustrated in Eq. (13), $|F_j|^2$ is a periodic function of $\bar{\tau}$, and so, with no loss in generality, $\bar{\tau}$ will be taken to be zero in which case $\bar{Q} = \pm \bar{q}$. Also, the Debye-Waller factors will be neglected since they are slowly varying functions of $\bar{q}$, and in addition, experimental evidence⁷ has indicated that W_0 is usually very similar to W_1 . Therefore, with the above assumptions, the structure factor becomes

$$\begin{aligned}
|F_j|^2 = q^2 \{ & \frac{[\hat{q} \cdot \bar{e}_0(\bar{q}, j)]^2 b_0^2}{M_0} \\
& + \frac{2[\hat{q} \cdot \bar{e}_0(\bar{q}, j)][\hat{q} \cdot \bar{e}_1(\bar{q}, j)] b_0 b_1}{\sqrt{M_0 M_1}} \\
& + \frac{[\hat{q} \cdot \bar{e}_1(\bar{q}, j)]^2 b_1^2}{M_1} \}
\end{aligned} \tag{15}$$

or

$$|F_j|^2 = q^2 |f_j|^2 \tag{16}$$

For $\underline{q}$ along high symmetry directions such as $[0\ 0\ 1]$, $[1\ 1\ 0]$ etc., both e_0 and e_1 are either parallel (longitudinal modes) or perpendicular (transverse modes) to $\underline{q}$. The reduced structure factors for these two cases are obtained by specifying the direction of $\underline{R} = (R_1, R_2, R_2)$ (which is discussed in the input data section) relative to $\underline{q}$.

D. Input data for the program

The input data cards are described below. In addition, comment cards in the program describe the input.

1st card: NFC, AMAS(1), AMAS(4), B0, B1. FORMAT (I5, 4F10.4).

NFC is the number of force constants appropriate to the model that is used to calculate the dynamical matrix elements. AMAS(1) and AMAS(4) are the masses (in atomic mass units) of the origin and body-centered atoms respectively. B0 and B1 are the coherent scattering lengths of the origin and body-centered atoms respectively.

2nd card: Q1, Q2, Q3, N1, N2, N3, M, IVEC, IFREQ, ISF. FORMAT (3F5.2, 7I1).

(Q1, Q2, Q3) designate the direction in reciprocal space along which the dispersion curves etc. are calculated. (N1, N2, N3) are parameters which

specify whether or not the respective (Q_1, Q_2, Q_3) values are allowed to vary. For example, if the dispersion curves are to be calculated along the $(\zeta \zeta 0)$ direction where

$$\zeta = q/q_{\max}, \quad (17)$$

then $Q_1 = 0.5$, $Q_2 = 0.5$, and $Q_3 = 0$ and $N_1 = 1$, $N_2 = 1$, and $N_3 = 0$. Alternatively, if the calculations are to be performed along the $(\frac{1}{2} \frac{1}{2} \zeta)$ direction, then $Q_1 = 0.5$, $Q_2 = 0.5$, and $Q_3 = 0.5$ and $N_1 = 0$, $N_2 = 0$, and $N_3 = 1$.

M is the number of points between $(0 \ 0 \ 0)$ and $(Q_1 \ Q_2 \ Q_3)$ at which the dispersion curves, for example, are calculated. That is, the program divides the length Q_1 into Q_1/M increments and calculates the desired quantities at M points along the interval. $IVEC$ is a parameter that controls the print-out of the atom polarization vectors e_0 , and e_1 . If $IVEC > 0$, the polarization vectors are printed out at each of the M points in the interval. If $IVEC$ is negative, they are not printed out. $IFREQ$ and ISF are analogous to $IVEC$ except that they control the print-out of the dispersion curves and the normalized structure factors respectively.

3rd card: R_1, R_2, R_3 . `FORMAT (3F5.2, 7I5).`

R_1, R_2 , and R_3 specify the direction of $\hat{q}$ in Eq. (14). For example, if the reduced structure factors for longitudinal phonons propagating in the $[0 \ 0 \ \zeta]$ direction are desired, then R_1, R_2 , and R_3 are 0, 0, and 1.0 respectively. For the transverse reduced structure factors R_1, R_2 , and R_3 are for example 0, 1.0, and 0 respectively.

4th card: PX(I). FORMAT (8F10.3).

The PX(I) are the interatomic force constants in dyne/cm. They are listed in the order

$$\alpha_1^1, \beta_1^1, \alpha_{10}^2, \alpha_{11}^2, \alpha_{20}^2, \alpha_{21}^2, \alpha_{10}^3, \alpha_{11}^3, \alpha_{30}^3, \alpha_{31}^3, \beta_{30}^3, \beta_{31}^3,$$

$$\alpha_1^4, \alpha_2^4, \beta_1^4, \beta_2^4, \alpha_{10}^5, \alpha_{11}^5, \beta_{10}^5, \beta_{11}^5, \alpha_{10}^6, \alpha_{11}^6, \alpha_{20}^6, \alpha_{21}^6.$$

The notation for the force constants is explained elsewhere.^{2,3}

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APPENDIX I

```
//S1      EXEC  FORTG,TIME.GO=01,REGION=96K
//FORT.SYSIN DD  *
      DIMENSION D(6,6),R(6,6),A(6,6),AA(21),RR(36),PX(24),AMAS(6),Q(3)
      DIMENSION S(12,3),C(12,3),U(3),W(6)
      EQUIVALENCE (R(1,1),RR(1))
C      THIS PROGRAM COMPUTES FOR THE CSCL STRUCTURE 1) POLARIZATION VECTORS
C      2) PHONON DISPERSION CURVES, 3) NORMALIZED STRUCTURE FACTORS FOR
C      INELASTIC NEUTRON SCATTERING
      READ 1, NFC,AMAS(1),AMAS(4),BO,B1
      1 FORMAT (I5,4F10.4)
      WRITE (3,1) NFC,AMAS(1),AMAS(4),BO,B1
C      NFC= THE NUMBER OF FORCE CONSTANTS
C      AMAS(1)= ATOMIC MASS OF ATOM AT ORIGIN
C      AMAS(4)=ATOMIC MASS OF ATOM AT (1,1,1)A/2
C      BO=SCATTERING LENGTH OF ORIGIN ATOM
C      B1=SCATTERING LENGTH OF ATOM AT (1,1,1)A/2
      WRITE(3,1)
      READ 2,Q1,Q2,Q3,N1,N2,N3,M,IVEC,IFREQ,ISF
      2 FORMAT (3F5.2,7I5)
      WRITE (3,2) Q1,Q2,Q3,N1,N2,N3,M,IVEC,IFREQ,ISF
      WRITE(3,1)
C      (Q1,Q2,Q3) DESIGNATE DIRECTION ALONG WHICH S.F. IS CALCULATED
C      NI SPECIFIES IF Q(I) VARIES
C      M IS THE NUMBER OF POINTS AT WHICH S.F. IS CALCULATED
C      IVEC SPECIFIES IF THE POLARIZATION VECTORS ARE PRINTED
C      IFREQ SPECIFIES IF THE FREQUENCIES ARE CALCULATED AND PRINTED
C      ISF SPECIFIES IF THE STRUCTURE FACTORS ARE CALCULATED AND PRINTED
      READ 2, R1,R2,R3
      WRITE(3,2) R1,R2,R3
C      (R1,R2,R3) IS A VECTOR EITHER PARALLEL OR PERPENDICULAR TO (Q1,Q2,Q3)
      READ 3,(PX(I),I=1,NFC)
      3 FORMAT (8F10.3)
      WRITE(3,1)
      WRITE(3,3) (PX(I),I=1,NFC)
      WRITE (3,1)
      PI=3.14159265
      U(1)=R1/SQRT(R1**2+R2**2+R3**2)
```

```

U(2)=R2/SQRT(R1**2+R2**2+R3**2)
U(3)=R3/SQRT(R1**2+R2**2+R3**2)
XMO=AMAS(1)
XM1=AMAS(4)
CPT=8.0*(PX(1)+PX(13)+2.0*PX(14))
AMAS(1)=1.0/SQRT(AMAS(1))
AMAS(2)=AMAS(1)
AMAS(3)=AMAS(1)
AMAS(4)=1.0/SQRT(AMAS(4))
AMAS(5)=AMAS(4)
AMAS(6)=AMAS(4)
DO 4 L=1,M
  IF (N1-0) 5,5,6
5  Q(1)=Q1
  GO TO 7
6  Q(1)=L*Q1/M
7  IF (N2-0) 8,8,9
8  Q(2)=Q2
  GO TO 10
9  Q(2)=L*Q2/M
10 IF (N3-0) 11,11,12
11 Q(3)=Q3
  GO TO 13
12 Q(3)=L*Q3/M
13 CONTINUE
  DO 14 I=1,3
    S(1,I)=SIN(PI*Q(I))
    C(1,I)=COS(PI*Q(I))
    S(2,I)=2.0*S(1,I)*C(1,I)
    C(2,I)=1.0-2.0*S(1,I)**2
    S(3,I)=S(2,I)*C(1,I)+S(1,I)*C(2,I)
    C(3,I)=C(2,I)*C(1,I)-S(1,I)*S(2,I)
14  C(4,I)=C(3,I)*C(1,I)-S(3,I)*S(1,I)
    DO 15 I=1,3
      IF(I-3) 17,16,17
16  J=1
    GO TO 18

```

```

17 J=I+1
18 IF(I-1) 19,20,19
20 K=3
   GO TO 21
19 K=I-1
21 D(I,I)=CPT+2.0*(PX(3)*(1.0-C(2,I))+PX(5)*(2.0-C(2,J)-C(2,K))
   A+2.0*(PX(7)*(2.0-C(2,I)*(C(2,J)+C(2,K)))+PX(9)*(1.0-C(2,J)
   B*C(2,K))+2.0*PX(17)*(1.0-C(2,I)*C(2,J)*C(2,K)))
   C+2.0*PX(21)*(1.0-C(4,I))+2.0*PX(23)*(2.0-C(4,J)-C(4,K))
   OD(I+3,I+3)=CPT+2.0*(PX(4)*(1.0-C(2,I))+PX(6)*(2.0-C(2,J)-C(2,K))
   A+2.0*(PX(8)*(2.0-C(2,I)*(C(2,J)+C(2,K)))+PX(10)*(1.0-C(2,J)
   B*C(2,K))+2.0*PX(18)*(1.0-C(2,I)*C(2,J)*C(2,K)))
   C+2.0*PX(22)*(1.0-C(4,I))+2.0*PX(24)*(2.0-C(4,J)-C(4,K))
   D(I+3,I)=-8.0*(C(1,J)*C(1,K)*(PX(1)*C(1,I)+PX(13)*C(3,I)))-8.0*
   A PX(14)*C(1,I)*(C(3,J)*C(1,K)+C(1,J)*C(3,K))
   D(I,I+3)=D(I+3,I)
   D(J,I)=4.0*PX(11)*S(2,I)*S(2,J)+8.0*PX(19)*S(2,I)*S(2,J)*C(2,K)
   D(I,J)=D(J,I)
   D(J+3,I+3)=4.0*PX(12)*S(2,I)*S(2,J)+8.0*PX(20)*S(2,I)*S(2,J)
   A*C(2,K)
   D(I+3,J+3)=D(J+3,I+3)
   D(J+3,I)=8.0*(S(1,I)*S(1,J)*(C(1,K)*PX(2)+PX(15)*C(3,K))+PX(16)*
   A C(1,K)*(S(3,I)*S(1,J)+S(1,I)*S(3,J)))
   D(J,I+3)=D(J+3,I)
   D(I+3,J)=D(J+3,I)
   D(I,J+3)=D(J+3,I)
15 CONTINUE
   DO 22 I=1,6
   DO 22 J=1,6
22 D(I,J)=D(I,J)*AMAS(I)*AMAS(J)
   DO 23 I=1,21
23 AA(I)=0.0
   AA(1)=D(1,1)
   AA(2)=D(1,2)
   AA(3)=D(2,2)
   AA(4)=D(1,3)
   AA(5)=D(2,3)

```

```

AA(6)=D(3,3)
AA(7)=D(1,4)
AA(8)=D(2,4)
AA(9)=D(3,4)
AA(10)=D(4,4)
AA(11)=D(1,5)
AA(12)=D(2,5)
AA(13)=D(3,5)
AA(14)=D(4,5)
AA(15)=D(5,5)
AA(16)=D(1,6)
AA(17)=D(2,6)
AA(18)=D(3,6)
AA(19)=D(4,6)
AA(20)=D(5,6)
AA(21)=D(6,6)
WRITE(3,1)
WRITE (3,1)
CALL EIGEN(AA,RR,6,0)
DO 25 I=1,21
  IF(AA(I)-0.0) 24,25,25
24 AA(I)=-AA(I)
25 CONTINUE
  IF (IVEC-1) 29,26,26
26 DO 27 I=1,6
27 WRITE(3,28) (R(I,J),J=1,6)
28 FORMAT (6E16.8)
  WRITE (3,1)
29 IF(IFREQ-1) 31,30,30
30 W(1)=SQRT(AA(1)/1.66043)/(2.0*PI)
  W(2)=SQRT(AA(3)/1.66043)/(2.0*PI)
  W(3)=SQRT(AA(6)/1.66043)/(2.0*PI)
  W(4)=SQRT(AA(10)/1.66043)/(2.0*PI)
  W(5)=SQRT(AA(15)/1.66043)/(2.0*PI)
  W(6)=SQRT(AA(21)/1.66043)/(2.0*PI)
  WRITE (3,28) (W(J),J=1,6)
31 IF(ISF-1) 4,32,32

```

```

32. DO 34 J=1,6
    S0=0.0
    S1=0.0
    S01=0.0
    SF=0.0
    QE0=0.0
    QE1=0.0
    DO 33 I=1,3
        QE0=QE0+U(I)*R(I,J)
33. QE1=QE1+U(I)*R(I+3,J)
        S0=(QE0*B0)**2/XM0
        S1=(QE1*B1)**2/XM1
        S01=2*(QE0*B0*QE1*B1)/SQRT(XM0*XM1)
        SF=(S0+S1+S01)
34. WRITE (3,1) L,SF
4. CONTINUE
END

```