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Investigation into the monotonic magnetostriction and magnetic breakdown in cadmium

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INVESTIGATIONS INTO THE MONOTONIC MAGNETOSTRICTION AND MAGNETIC BREAKDOWN IN CADMIUM

by

JAMES MILO CARTER, 1944-

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ABSTRACT

Observations of the monotonic magnetostriction of cadmium at 4.2 K and in fields of 65 kilogauss have been made. The angular dependence of an extremal point \( H_m \) in the monotonic magnetostriction is found to follow inverse cosine behavior. The magnitude of \( H_m \) (27 kG) for fields parallel to [0001] is in fair agreement with the onset of \( \gamma_{1/3} \) from the breakdown of the trifoliate orbit, \( \gamma \). The range of observation of \( H_m \) coincides with the reported range of the trifoliate orbit. A "kink" in the monotonic magnetostriction is demonstrated. The "kink" field, \( H_k \), is constant in value at 23 kilogauss to 60° from the c axis in a \{10\overline{1}0\} plane.
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## TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>ii</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>v</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. EXPERIMENTAL DETAILS</td>
<td>5</td>
</tr>
<tr>
<td>III. THEORY</td>
<td>6</td>
</tr>
<tr>
<td>A. Monotonic</td>
<td>6</td>
</tr>
<tr>
<td>B. Oscillatory</td>
<td>8</td>
</tr>
<tr>
<td>IV. PRESENTATION OF RESULTS</td>
<td>10</td>
</tr>
<tr>
<td>A. Magnetostriction</td>
<td>10</td>
</tr>
<tr>
<td>B. Magnetization</td>
<td>20</td>
</tr>
<tr>
<td>C. Summary</td>
<td>21</td>
</tr>
<tr>
<td>V. DISCUSSION</td>
<td>24</td>
</tr>
<tr>
<td>VI. APPENDICES</td>
<td>29</td>
</tr>
<tr>
<td>A. Expanded Discussion of Experimental Details</td>
<td>29</td>
</tr>
<tr>
<td>1. Magnetostriction</td>
<td>29</td>
</tr>
<tr>
<td>2. Magnetization</td>
<td>35</td>
</tr>
<tr>
<td>3. Calibration of x-y recorder</td>
<td>38</td>
</tr>
<tr>
<td>B. Sample Preparation</td>
<td>41</td>
</tr>
<tr>
<td>C. Fourier Transforms of Simple Cases</td>
<td>43</td>
</tr>
<tr>
<td>D. Non Linear Least Squares</td>
<td>47</td>
</tr>
<tr>
<td>E. Computer Program Used in Analysis</td>
<td>50</td>
</tr>
<tr>
<td>1. Description of program</td>
<td>50</td>
</tr>
<tr>
<td>2. Definition of symbols and program listing</td>
<td>56</td>
</tr>
<tr>
<td>VII. BIBLIOGRAPHY</td>
<td>84</td>
</tr>
<tr>
<td>VIII. VITA</td>
<td>87</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figures</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Magnetostriction parallel to c-axis.</td>
<td>11</td>
</tr>
<tr>
<td>2. Magnetostriction parallel to a basal plane direction.</td>
<td>12</td>
</tr>
<tr>
<td>3. Magnetostriction parallel to [0001] ( H^2 ) vs ( H^2 ).</td>
<td>13</td>
</tr>
<tr>
<td>4. Magnetostriction parallel to [1120] ( H^2 ) vs ( H^2 ).</td>
<td>14</td>
</tr>
<tr>
<td>5. Characteristics observed in the monotonic magnetostriction.</td>
<td>16</td>
</tr>
<tr>
<td>6. Coefficient of ( H^2 ) for low field expansion.</td>
<td>19</td>
</tr>
<tr>
<td>7. Onset of magnetic breakdown of trifoliate orbit.</td>
<td>22</td>
</tr>
<tr>
<td>8. Difference between low field and high field coefficients of ( H^2 ) and ( H^4 ).</td>
<td>27</td>
</tr>
<tr>
<td>A1. Schematic representation of magnetostriction cell.</td>
<td>30</td>
</tr>
<tr>
<td>A2. Schematic of electrical circuitry for measuring magnetostriction.</td>
<td>33</td>
</tr>
<tr>
<td>A3. Schematic representation of modulation probe.</td>
<td>37</td>
</tr>
</tbody>
</table>
Investigations Into the Monotonic
Magnetostriction and Magnetic
Breakdown in Cadmium

I. INTRODUCTION

Magnetostriction, or field dependent strain, is the change in the dimensions of a sample arising from the magnetization of the sample. Magnetostriction can be defined by \([L(H)-L(0)]/L(0)\) where \(L(H)\) is the field dependent length for a dimension of the sample. In general a crystal has six components of strain; three longitudinal strains parallel to, and three shear strains perpendicular to the major crystallographic symmetry directions.

Though magnetostriction was discovered in iron by Joule\(^1\) in 1847, the first observation of the monotonic magnetostriction (MM) in a nonferromagnetic material, viz., diamagnetic Bi, was reported by Kapitza\(^2\) in 1932. Shoenberg\(^3\) continued the study of Bi under the direction of Kapitza. Little further work has been reported on the MM of nonferromagnetic materials since 1934.

Chandrasekar pointed out that magnetostriction oscillatory in \(1/H\) should exist by consideration of the oscillatory free energy.\(^4\) This effect depends upon the stress dependence of the area of the extremal orbits of the Fermi surface. Chandrasekar's paper was notable as the first successful
association of a microscopic theory with magnetostriction observations. This paper will be concerned chiefly with the observations of the anomalous monotonic magnetostriction of cadmium. There will be attempts to relate these observations to known effects in the oscillatory susceptibility (OS).

The free electron theory of metals predicts that, since the Landau diamagnetism is \(-1/3\) the Pauli spin paramagnetism, all metals should be paramagnetic. In fact many polyvalent metals are diamagnetic. This is thought to arise as a consequence of a small number of charge carriers having very small effective mass. The Landau-Peierls diamagnetic susceptibility is thus increased because of the large components of the reciprocal mass tensor. Such small mass may also allow for interband, magnetic field induced coupling across the associated small band gaps.

E. N. Adams performed a model calculation for a two band model near a Brillouin zone boundary allowing for interband coupling due to an applied magnetic field. Such fields usually lead to negligible mixing of bands, but a large second order energy correction term can arise for small band gaps. Adams' derivation for the anomalous susceptibility evaluated for zero field gave, in addition to the usual Landau-Peierls diamagnetic term, a term which could be positive or negative and very large in comparison to the Landau-Peierls term.

A calculation of the diamagnetic susceptibility of the conduction electrons in metals as presented by Hebborn and
Sondheimer\textsuperscript{6} continued the density matrix approach by expanding the partition function to order $H^2$. This led to a difficult and complicated result due to the non-periodicity of the magnetic field. Hebborn, Luttinger, Sondheimer, and Stiles\textsuperscript{7} greatly simplified this derivation by superimposing a periodic field and letting the period go to infinity at the end of the calculations. Their result is still extremely complicated. A pseudopotential approach was recently employed by Misra and Roth\textsuperscript{8} to calculate the diamagnetic susceptibility of conduction electrons in polyvalent metals. While far from transparent, their result is most nearly related to this experiment.

The theory for the monotonic susceptibility of nonferromagnetic materials is not as detailed as the theory for the oscillatory effects. The Maxwell relationship $\partial \varepsilon / \partial H = \partial M / \partial \sigma$ relates the magnetization, $M$, to the magnetostriction, $\varepsilon$, through the magnetic field, $H$, and the stress, $\sigma$. Further information is gained when a stress-dependent magnetization can be calculated from the Fermi surface properties. This calculation seems impractical due to its dependence on the periodic, $u_{nk}(r)$, part of the Bloch functions.

In contrast the Lifshitz-Kosevich\textsuperscript{9} (LK) thermodynamic potential for the oscillatory part of the free energy accurately describes the period, temperature, and field dependence of the oscillatory effects. This theoretical expression has been corrected for spin orbit splitting,\textsuperscript{10} non-thermal scattering,\textsuperscript{11} and the phenomenon of magnetic break-
down. The period, temperature dependence, and field dependence of this function relate directly to the Fermi surface morphology, and accurately predict the oscillatory magnetostriction.

The presently accepted model of the Fermi surface of cadmium is the orthogonalized-plane-wave surface arising from a non-local pseudopotential as calculated by Stark and Falicov. The terminology for the pertinent orbits (areas) will be that of Tsui and Stark. Other relevant papers on the band structure of cadmium are listed as references 15-18.
II. EXPERIMENTAL DETAILS\textsuperscript{19}

The work reported in this paper was done at temperatures between 1.3 and 4.2 K and in applied fields to 65 kG. The OS was measured using low frequency field modulation techniques similar to, but simpler than, those described by Stark and Windmiller.\textsuperscript{20} The magnetostriction data were taken using a three terminal capacitance method similar to that used by White\textsuperscript{21} for thermal expansion measurements. Sample orientations were determined by standard Laue techniques. The samples were cut with a spark cutter.\textsuperscript{22} The magnetic field of the superconducting solenoid was calibrated using known de Haas-van Alphen (dHvA) frequencies in Be.\textsuperscript{23}

Magnetostriction data were recorded as \( C(H) \) where \( C \) is the unbalance capacitance of a capacitance bridge. This recording is converted to strain using the relationship for strain, \( \varepsilon = \Delta L / L_0 = \Delta d / L_0 = \frac{[C(H) - C(0)]d}{C(0)L_0} \) where \( L_0 \) is the zero field length of the crystal, \( d \) is the gap spacing in the capacitor, and \( C \) is the capacitance of the cell as a function of applied field.
III. THEORY

A. Monotonic

Magnetostriction can be thought of as a change in the shape of a crystal which lowers its free energy when it becomes magnetized. To describe the magnetostriction of a body, let us choose as independent variables the temperature, T, the six components of stress, \( \sigma_a \) (\( a=1,2,3,4,5,6 \)), and the three components of the magnetic field, \( H_a \) (\( a=1,2,3 \)). We take \( U \) as the thermodynamic potential per unit volume of the body to be a function of these variables; \( U = f(T, H, \sigma) \). For a body having no permanent magnetization and having inversion symmetry, the magnetostriction will be symmetric with reversal of the field. For isothermal processes, the potential, \( U \), can be expanded in even powers of the applied field and in all powers of the crystalline stress.

It can be shown that the magnetostriction may be written as

\[
\varepsilon_{\alpha} = 0.5m_{ab,\alpha}H_aH_b + 0.25m_{abcd,\alpha}H_aH_bH_cH_d + \cdots 
+ 0.25m_{ab,\alpha\beta}H_aH_\beta + \text{h.o.t.} 
\]  

(1)

The Einstein summation convention is used, i.e. repeated indices are summed. The \( m \)'s of this equation are atomic moduli of magnetostriction and are temperature dependent. Equation (1) is to be evaluated for \( \sigma=0 \) as the crystal produces negligible stress on its environment in these experi-
ments. The MM at constant temperature will thus be a function of even powers of the applied field.

This equation is used in an equivalent form. One can write Eq. (1) for the strain measured in the direction of the applied field as

\[ \varepsilon_{11} = m_{11}a H^2/2 + m_{1111}a H^4/4 + m_{111111}a H^6/6 + \text{h. o. t.} \]

\[ = AH^2 + BH^4 + \text{Ch}^6 + \text{h.o.t.} \] (2)

When the strain is measured in a direction perpendicular to the applied field, the equation can be written as

\[ \varepsilon_\perp = (m_{11}a H_1^2 + 2m_{12}a H_1 H_2 + m_{22}a H_2^2)/2 + \text{h.o.t.} \] (3)

where \( H_1 \) and \( H_2 \) are the components of the magnetic field in two symmetry directions of the crystal. Let \( H \) be the magnitude of the applied field and \( \theta \) the angle between the direction of the applied field and the highest symmetry direction in the plane of interest. Write \( H_1 = H \cos \theta \) and \( H_2 = H \sin \theta \).

Inserting these two expressions into Eq. (3) one gets

\[ \varepsilon_\perp = (m_{12}a \cos^2 \theta + m_{22}a \sin^2 \theta + m_{22}a \sin^2 \theta)H^2/2 + \text{h.o.t.} \] (4)

Now rename the coefficients of the successive powers of \( H^2 \) so that the expression for the magnetostriction becomes

\[ \varepsilon_\perp = a(\theta)H^2 + b(\theta)H^4 + c(\theta)H^6 + \text{h.o.t.} \] (5)

where

\[ a(\theta) = (m_{11}a \cos^2 \theta + m_{12}a \sin^2 \theta + m_{22}a \sin^2 \theta)/2 \] (6)
with similar but more complicated expressions for \( b(\theta) \), \( c(\theta) \), etc. This form of the expansion, Eq. (5) was used to fit the data.

B. Oscillatory

The oscillations in the free energy which give rise to oscillations in the susceptibility, i.e. the dHvA effect, also give rise to oscillations in the magnetostriction as a function of field. The LK expression for the oscillatory free energy without magnetic breakdown (MB) can be found in many references.

The problem of modifying the LK expression for the field dependence of the dHvA effect in the presence of MB has been considered extensively. The expression for the probability of breakdown at any corner (Bragg reflection) of an electron orbit is given by

\[
P = \exp\left(-H_0/H\right)
\]

where \( H_0 \) is given by

\[
H_0 = \frac{\pi V_G^2}{4R} |v_x v_y|
\]

Here \( V_G \) is the energy gap thru which tunneling occurs, \( G \) is a wave vector defining the Brillouin zone boundary, \( H \) is parallel to the zone face defined by \( G \) and is in the \( z \) direction, and \( v_x \) and \( v_y \) are the normal and tangential components of the free electron velocity at the zone face.
Chambers$^{29}$ clarified the analytical work of Pippard$^{31}$ by using a model calculation for a three corner orbit. The trifoliate orbit in cadmium is such a three corner orbit and is similar to the needle orbit in zinc$^{32}$ turned inside out. For this model Chambers found as the correction for the $j$th harmonic in the oscillatory free energy

$$B_j = [1 - \exp(-H_0/H)]^{3j/2} = |q|^{3j}$$

(9)

where

$$|q|^2 = 1 - |p|^2 = 1 - P.$$  

(10)

For field directions away from the $c$ axis, the Green's function approach of Falicov and Stachowiak$^{33}$ may be more appropriate as it gives a $q_1q_2q_3$ product dependence for the breakdown correction. In all cases, the leading term in the angular variation of $H_0$ is inverse cosine.
IV. PRESENTATION OF RESULTS

A. Magnetostriction

Figures 1 and 2 are tracings of x-y recorder plots of the field dependent strain (magnetostriction), \( \varepsilon(H) \), vs applied field, \( H \), for two principal symmetry directions in admium at 4.2 K. The oscillations appearing in these tracings are due to the dHvA effect and will not be considered in this paper. The baseline, monotonic magnetostriction, will receive primary consideration, although some relevant observations of the OS are included.

The strain, as given by Eq. (5), is a polynomial in \( H^2 \). The data shown in Figs. 1 and 2 were divided by \( H^2 \) and plotted against \( H^2 \) as Figs. 3 and 4. This allows one to read from the intercept the coefficient of \( H^2 \), from the slope the coefficient of \( H^4 \), and from the quadratic curvature the coefficient of \( H^6 \), if any. No terms higher than sixth order in \( H \) appear in these data.

If the value of \( C(0) \), the capacitance at zero field, is read in error by one half the least division of the recorder paper, the curve of \( \varepsilon/H^2 \) diverges as shown by the error bars in Figs. 3 and 4. (This is just the divergence of \( \Delta C(0)/X \) as \( X \) goes to zero.) The value of \( C(0) \) was chosen to give the best straight line fit on this plot as \( H^2 \) goes to zero.

It is apparent that a single expansion does not adequately fit the MM data of Figs. 3 and 4. Two independent expansions of the form indicated in Eq. (5) fit this data
MAGNETOSTRICTION PARALLEL TO C-AXIS. A plot of the magnetostriction along the c axis as a function of the applied field parallel to the c axis. The high field portion shows a shortening of the crystal and de Haas-van Alphen type oscillations.
Figure 1

\[ \text{STRAIN} = 2.53 \times 10^{-7} \]
FIGURE 2

MAGNETOSTRICTION PARALLEL TO A BASAL PLANE TION. A plot of the magnetostriction parallel as a function of the applied field parallel to axis. The high field portion shows a lengthened crystal and de Haas-van Alphen type oscillation
STRAIN = $1.28 \times 10^{-7}$
The magnetostriction, $\varepsilon$, divided by $H^2$ and plotted against $H^2$ to show the "kink" in the expansion at 25 kG. This is the data of Fig. 1, $\varepsilon||[0001]$ and $H||[0001]$. The error bars near the origin represent the effect of plus or minus one smallest division scale error in choosing $\varepsilon_0$, the zero of the strain scale. The expansions for the two solid curves are $\varepsilon_L = 4.4 \times 10^{-16} H^2 - 2.8 \times 10^{-25} H^4$ and $\varepsilon_H = 7.5 \times 10^{-16} H^2 - 7.9 \times 10^{-25} H^4 + 1.2 \times 10^{-34} H^6$ for $H$ in gauss.
FIGURE 4

MAGNETOSTRICTION PARALLEL TO (11\overline{2}0)/H^2 VS H^2.
The magnetostriction, \( \varepsilon \), divided by \( H^2 \) and plotted against \( H^2 \) to show the "kink" in the expansion at 25 kG. This is the data of Fig. 2, \( \varepsilon ||[11\overline{2}0] \) and \( H||[0001] \). The error bars near the origin represent the effect of plus or minus one smallest division scale error in choosing \( \varepsilon_0 \), the zero of the strain scale. The expansions for the two solid curves are

\[ \varepsilon_L = -2.5 \times 10^{-16} H^2 + 1.4 \times 10^{-25} H^4 \]

and

\[ \varepsilon_H = -4.2 \times 10^{-16} H^2 + 5.0 \times 10^{-25} H^4 - 6.6 \times 10^{-35} H^6 \] for \( H \) in gauss.
Figure 4
very well when applied above and below 625 kG. The intersection of the low field expansion and the high field expansion defines a "kink" field, $H_k$.

Another feature of the MM data is the existence of a field for which the slope of $\varepsilon(H)$ is zero. Since the relevant Maxwell relation is $\partial \varepsilon / \partial H = \partial M / \partial \sigma$, this field marks the boundary of a field induced sign change in the stress dependent derivative of the magnetization. We denote this field by $H_m$.

The value of $H_k$ is equal to the value of $H_m$ for the data sets of Figs. 1 and 2 and is near 25 kG. Magnetic breakdown of the trifoliate orbit in cadmium is known to occur at about 25 kG for fields along the c axis. An angular study was done to see if either of these two features, $H_k$ or $H_m$, could be associated with the inverse cosine behavior of the breakdown effect.

This angular study was taken for the field in a $\{1010\}$ plane and the strain along a $<10\bar{1}0>$ direction. The sample used was cut from a different boule than the samples of Figs. 1 and 2. The results for $H_m$ and $H_k$ are displayed in Fig. 5 with $H_m$ represented by the small triangles and $H_k$ by the open circles.

Examination of Fig. 5 shows that there is little or no angular variation to $H_k$. The horizontal dashed line represents the average for $H_k$, which is 23 kG. These values of $H_k$ were read from plots of $\varepsilon/H^2$. The kink is observable in the data out to an angle of at least 60° from the c axis. Beyond
FIGURE 5

CHARACTERISTICS OBSERVED IN THE MONOTONIC MAGNETOSTRICTION. Characteristic values of the applied magnetic field plotted against orientation of magnetic field in a \{10\bar{1}0\} plane. The diamond at the left margin marks the onset of $\gamma_{1/3}$. The square marks the value for the kink field of Figs. 3 and 4, as well as the value for which $\partial \varepsilon / \partial H = 0$. The circles about the horizontal line indicate the kink field for transverse strain measurements with the magnetic field in a \{10\bar{1}0\} plane. The small triangles indicate the magnetic field strength for $\partial \varepsilon / \partial H = 0$, i.e. $H_m$ where the inverted triangles have been folded about \[11\bar{2}0\]. The vertical dashed line shows the range of the trifoliate orbit, $\gamma$, in this plane. The large triangle on the right represents the breakdown field of the arm and cap gap at $H$ in the Brillouin zone. The solid curve is inverse cosine normalized to 27 kG.
Figure 5
this angle a single expansion would fit the data as well as, or better than, two expansions. The range of $H_k$ is in approximate agreement with the angular range of the trifoliate orbit as an extremal orbit centered at $K$.\textsuperscript{14} The reported range of $\gamma$ of 69.5° in this plane is indicated by the vertical dashed line in Fig. 5. One notes that $H_k$ lies between the values for the breakdown of the trifoliate orbit in the basal plane and the value for breakdown reported by Daters and Cook of the spin orbit gap near L.\textsuperscript{34}

The extremal field, $H_m$, exhibits an angular dependence as shown in Fig. 5. The inverted triangles, $\nabla$, have been folded about [1120]. Symmetry demands that these folded points fall on the unfolded ones. It was learned after this data had been taken that the sample was oriented slightly away from [1100] toward [0001] which may account for the slight discrepancy. The +'s connected by a solid line are a plot of $\sec \theta$ normalized to the value of $H_o = 27$ kG. This value for $H_o$ will be shown in the next subsection to be approximately the breakdown field of the trifoliate orbit in these samples. The value of $H_m$ is different in this sample than in those giving the data displayed in Figs. 1 and 2. This is attributed to the samples having been cut from different boules.\textsuperscript{35}

A computer program was used in the analysis of the magnetostriction data. The program averaged the data to remove the oscillatory magnetostriction. A low field and a high field regime are defined for the data and separated by $H_k$. Although the expression for the MM does not have a constant
term \((c=0 \text{ at } H=0 \text{ by definition})\), allowance was made in both the low field expansion and the high field expansion to include such a term. The reason for including the constant term in the low field expansion is to make allowance for not selecting the proper zero value for the strain scale. The high field constant term was included to see if the least squares fit duplicated the low field value of the zero field sample length.

This constant term, \(C(0)\), in the high field expansion did not usually duplicate the low field value. Close to the \(c\) axis its value indicated a small difference \((10^{-7})\) in the zero field length of the sample between the high field and the low field values. This difference in zero field length smoothly approaches zero as the field is tilted from the \(c\) axis.

As a check to see if a single expansion could be forced to fit these data, a fit to the entire range of the data was done to the same order polynomial as used for the high field fit. The calculated standard deviation for this fit was larger than that for the low field or high field by an order of magnitude in the majority of the field sweeps examined for \(H\) within 60° of the \(c\) axis.

A plot of \(a_{LF}(\theta)\), the coefficient of \(H^2\), for the low field fit to the data is shown in Fig. 6. The calculated variance for each datum is the size of the plotted points. The variance of the coefficient is therefore much less than the scatter in the magnitude of the coefficient. This
FIGURE 6

COEFFICIENT OF $H^2$ FOR LOW FIELD EXPANSION.

A plot of the low field coefficient of $H^2$ for magnetostriction measurements in a ($10\bar{1}0$) direction with the field in a ($10\bar{1}0$). $\theta$ measures the angle between the applied field and the c axis. The dashed curve represents $\Delta\cos^2\theta$ as expected from classical thermodynamics. This coefficient begins to deviate from this behavior near $60^\circ$ and begins to oscillate in sign near [1120]. This is not shown as the amplitude is small. The vertical dashed line at $69^\circ$ marks the limit of the trifoliate orbit in this plane.
\begin{figure}
\centering
\includegraphics{figure6.png}
\caption{Figure 6}
\end{figure}
situation has not been satisfactorily explained. However, it is not thought to be an artifact of the analysis. The average value of this coefficient seems to be changing in a smooth manner to an angle of approximately $65^\circ$ from the c axis at which point it begins to drop faster than $\cos^2 \theta$. The sign of $a_{LF}$ begins to oscillate $13^\circ$ from [1120].

Examination of Eq. (6) will show that the $\theta$ dependence of this coefficient is a smooth function of angle for an expansion in constant coefficients $m_{ijk}$. The expected behavior is shown as the dashed line in Fig. 6 ($A\cos^2 \theta$). The observed angular dependence is as expected from the classical thermodynamics used to derive Eq. (5). The oscillation of the sign of the coefficient for field directions near [1120] is unexpected however. A similar behavior was observed in the coefficient of $H^4$ in the low field expansion. The results for the low field coefficient of $H^4$ shows that it has a leading term of $\cos^4 \theta$. The high field coefficients also followed a smooth function over the angular range for which they were definable.

B. Magnetization

To determine whether the angular variation of $H_m$ could be related to MB, $dHvA$ studies were done on samples cut from the same boule as the magnetostriction sample used in the angular study. These samples were cut for susceptibility measurements of $\chi$ parallel to $H$, at angles of 0, 20, and 35
degrees from the c axis toward [10\bar{1}0] in a \{11\bar{2}0\} plane.

The trifoliate orbit, γ, breaks into two orbits, \(γ_{1/3}\) and \(γ_{2/3}\), for fields along the c axis. The onset of \(γ_{1/3}\) was seen at approximately 27 kG for \(H\parallel[0001]\). This observation of the onset of \(γ_{1/3}\) is shown in Fig. 7. The estimate of 27 kG is made from the extrapolation of the modulation above 28 kG to an intersection with the baseline of the data below 28 kG.

For each of the three orientations chosen, frequency terms were found in the data which correspond to what might be called \(γ_{1/3}\) and \(γ_{2/3}\) as well as γ. Away from the c axis the trifoliate orbit does not separate into two areas in the ratio of 2:1 as it does for \(H\) along the c axis. The onset of the subharmonics of γ was observed at 30 kG for \(H\) 20° from the c axis and 32 kG for \(H\) 35° from the c axis. These values of \(H_o\) agree substantially with the value of \(H_m\) at the same angles.

C. Summary

These experimental observations may be summarized as follows:

1) The extrema of the monotonic magnetostriction, \(H_m\), vary with angle of the applied field from the c axis closely as \((\cosθ)^{-1}\). These extrema are observable to about 65° from the c axis in fields to 65 kG.
ONSET OF MAGNETIC BREAKDOWN OF TRIFOLIATE ORBIT. The susceptibility, $\chi$, parallel to $H$ and parallel to the c axis in cadmium at 1.3 K. This shows the onset of $\gamma_{1/3}$ orbit at approximately 27 kilogauss.
Figure 7

SUSCEPTIBILITY

28 kG
ONSET \( \gamma_{1/3} \) (4.8 \( \times \) 10\(^{-8}\) g\(^{-1}\))

H (kG)

27 29 31
2) There is a "kink" field, \( H_k \), which exists in the data to an angle of at least 60° from the c axis. The angular variation of the expansion coefficients begin to show slight deviations from simple \( \cos^2 \Theta \) or \( \cos^4 \Theta \) dependence in this angular range.

3) The oscillatory susceptibility has frequency terms which add to give the published value of the trifoliate orbit. The estimated value of \( H_o \) for \( H||[0001] \) agrees reasonably well with that of Tsui and Stark, allowing for the higher purity of their sample.
V. DISCUSSION

Calculations for the anomalous susceptibility of a two band model indicate that a peak in the susceptibility occurs just as the Fermi energy coincides with a band extremum.\textsuperscript{5,36} This has been observed for cadmium at 6.5\% Mg and 4.2 K, indicating the passage of the needle (third band electrons) through the Fermi energy as c/a is varied by alloying. Similar effects have been noted in alloy studies of bismuth and indium.\textsuperscript{37} Population of low lying bands by thermal excitation or by thermal expansion changes in c/a is thought to be responsible for peaks in the temperature dependent susceptibility of zinc,\textsuperscript{37} bismuth,\textsuperscript{37} and cadmium alloys with magnesium.\textsuperscript{36} It is proposed that magnetic breakdown from the second band arm to the first band cap serves to populate the cap near its saddle point (van Hove singularity) with an effect equivalent to applied stress or increased temperature.

The experimental evidence, while circumstantial, points strongly to MB from the region of the trifoliate orbit near K through the caps.\textsuperscript{14} The magnitude of $H_m$ agrees closely with the observation of the onset of $\gamma_1/3$ at the c axis. The angular variation of $H_m$ is closely that of $(\cos \theta)^{-1}$, as expected for MB fields. The value of $H_m$ moves to higher fields with increasing temperature.\textsuperscript{38} The value of $H_m$ observed at the c axis is lower for higher purity crystals, i. e., it increases with increasing temperature independent scattering (the Dingle temperature).\textsuperscript{11} The range of observation of $H_m$ coincides with the range of $\gamma$.\textsuperscript{14}
It is tempting to conclude that $H_m$ is directly associated with MB. However, consider the following classical argument. The low field portion of the MM fits the function $y = aH^2 + bH^4$. This function has an extremal

$$H_E = (-a/2b)^{1/2}. \tag{11}$$

The sign of $a$ and $b$ are opposite, thus minimizing the volume magnetostriction. The coefficient $a$ varies as $\cos^2 \theta$ and the coefficient $b$ varies as $\cos^4 \theta$, scaled by the constant coefficients $m_{\text{iiik}}$ and $m_{\text{iiiiik}}$. Thus, the calculated extremal, $H_E$, of the low field fit should vary as $(\cos \theta)^{-1}$. The magnitude of the calculated low field extremal lies outside the field range defining the low field regime.

The high field expansion is expected to have an extremal field value which also goes as $(\cos \theta)^{-1}$. The high field extremal falls within the range of $H$ defining the high field regime. The calculated value of $H_E$ in the high field region, using the high field coefficients $a_{HF}$ and $b_{HF}$, duplicates the triangles of Fig. 5, i.e. $H_m$, as expected. The extremal of the MM closely follows the prediction of classical thermodynamics.

If the sixth order term in the high field expansion and the constant terms, $Y_0$, (previously called $C(0)$), are neglected for simplicity, $H_k$ is defined by

$$a_{LF}H_k^2 + b_{LF}H_k^4 = a_{HF}H_k^2 + b_{HF}H_k^4$$
\[ H_k^2 = \frac{(a_{HF} - a_{LF})}{(b_{LF} - b_{HF})} \quad (12) \]

\[ = H_E^2 \frac{a_{LF}/a_{HF} - 1}{1 - b_{LF}/b_{HF}}. \quad (13) \]

All like coefficients have the same dominant angular variation, i.e. \( a_i \propto \cos^2 \theta \) and \( b_i \propto \cos^4 \theta \). The ratios of \( a_i/a_j \) and \( b_i/b_j \), to a first approximation, are angular independent. The ratios of \( a_i/b_i \), or \( H_E \) from Eq. (11), will have a \((\cos \theta)^{-2}\) dependence. Hence, \( H_k \) should vary as \((\cos \theta)^{-1}\) according to Eq. (13). That it doesn't is obvious from Fig. 5.

A plausible explanation of the lack of any obvious angular variation of the "kink" field is as follows: The constant kink field implies that either the numerator or denominator of Eq. (12) does not follow the angular variation indicated by the classical theory and demonstrated in Fig. 6 for the low field coefficient, \( a_{LF} \), of \( H^2 \). Figure 8 shows \( |a_{HF} - a_{LF}| \) and \( |b_{HF} - b_{LF}| \) as a function of angle. The superposition of the function \( A \cos^4 \theta \) shows that each of these difference functions varies approximately as \( \cos^4 \theta \).

The angular variation of \( a_{LF} \) or \( a_{HF} \) as given by Eq. (5) may be approximated by \( a_{LF} = m_{11} \cos^2 \theta \) and \( a_{HF} = m_{11}' \cos^2 \theta \), since \( m_{11} \) is the dominant coefficient. A factor of 1/2 and a subscript have been suppressed. Figure 6 shows that \( a_{LF} \) does in fact vary as \( \cos^2 \theta \) with \( m_{11} \) constant. The variation in \( a_{HF} \) is not as clearly determined and may contain angular dependence in \( m_{11}' \). That \( m_{11}' \) is angular dependent is shown by comparing the angular variation of the difference of the low field and high field coefficients of \( H^2 \) to the demon-
DIFFERENCE BETWEEN LOW FIELD AND HIGH FIELD

COEFFICIENTS OF $H^2$ AND $H^4$. a) Shows that the difference of $a_{HF} - a_{LF}$ follows a $\cos^4 \theta$ dependence. The solid curve is $5 \times 10^{-16} \cos^4 \theta$. This $\cos^4 \theta$ is not expected by the classical thermodynamic results. b) Shows the difference $b_{HF} - b_{LF}$ which seems to follow the $\cos^4 \theta$ variation as expected. The solid curve is $5 \times 10^{-25} \cos^4 \theta$. Both of these difference functions seem to vanish near $70^\circ$ from the c axis which is the range of the trifoliate orbit in the (1010) plane.
Figure 8
strated angular dependence of the low field coefficient and the assumed angular dependence of the high field coefficient. This allows one to solve for the angular behavior of the high field coefficient of $H^2$. This may be written as

$$a_{HF} - a_{LF} = m_{11} \cos^2 \theta - m_{11} \cos^2 \theta = A \cos^4 \theta$$

$$m_{11}' \cos^2 \theta = m_{11} \cos^2 \theta + A \cos^4 \theta$$  \hspace{1cm} (14)

$$m_{11}' = m_{11}(1 + f \cos^2 \theta)$$ \hspace{1cm} (15)

which shows that the coefficient of $H^2$ in the high field regime is not constant but is angle dependent. This effect may also occur in the high field coefficient of $H^4$ but it is not apparent in these data.

Figure 8 and Eq. (12) give a value of 32 kG for the kink field in contrast to the 23 kG displayed in Fig. 5. This difference can be attributed to the approximations made in writing Eq. (12). The value of 23 kG as determined from the plots of $\varepsilon/H^2$ vs $H^2$ is the better value for the kink field.

A self-consistent picture could be formed if it were shown theoretically that the filling of hole-type, saddle-point states lying just under the Fermi level gave rise to paramagnetic contributions to the susceptibility. In that case, the anomalous magnetostriction in cadmium would be shown to be due to interband coupling (or MB) by the magnetic field of the same bands as those of the anomalous susceptibility.
VI. APPENDICES

A. Expanded Discussion of Experimental Details

1. Magnetostriction

A three terminal, guard ring, capacitance technique was used to measure the magnetostriction. This is an adaption of the technique used by White\textsuperscript{21} for thermal expansion measurements. In this technique the length change of the sample is compared to the length change of the capacitance cell body reference material. The cell should have magnetostriction one or two orders of magnitude below that of the sample in the ideal case. The thermal expansion of the cell reference material should match that of the sample, if possible. Berylco 25 was used as the cell material in this work since it exhibits no quantum effects, is non-magnetic, and has low thermal expansion and magnetostriction at liquid helium temperatures.

A schematic representation of the cell is shown in Fig. A1. The top plate, formed by parts 2, 3, and 8, is considered as the fixed, guarded plate of the guard-ring parallel plate capacitor. This top plate consists of the guard ring (8), an epoxy coated mylar sheet forming an insulator between the guard-ring and the central electrode (3), and the central electrode (2). A mylar spacer (4) is used to set the gap for the capacitor. The sample (6) provides the movable plate of the capacitor.
Fig. A1. Schematic representation of magnetostriction cell. The parts are: 1 - electrical lead terminals, 2 - central electrode of the top plate, 3 - mylar and epoxy insulator, 4 - mylar washer for gap spacing, 5 - cell body, 6 - sample, 7 - pedestal in bottom plate or sample mount, and 8 - outer ring of top and bottom plate.
After the epoxy insulator and "plug" have been inserted into the ring, one side of the resulting assembly is lapped flat and provides a top plate of a cell. If the assembly is to be used as a bottom plate, a pedestal is left on one side for mounting the sample. A small tip is left on the opposite (or out) side for attachment of an electrical lead on both the top and bottom plates. Part (5) is the cell body, or reference frame. An assembled cell is 0.535 inches in diameter and approximately 0.75 inches in length.

The expression for the capacitance for a circular parallel plate capacitor corrected for fringing effects can be written as

\[ C = \frac{\varepsilon \pi r^2}{4d} + \frac{\varepsilon \pi w}{d+0.22w} \left(1+\frac{w}{2r}\right) \text{esu (cgs-cm)}. \] (A-1)

In this expression \( \varepsilon \) is the dielectric constant, \( r \) is the radius of the top central electrode, \( d \) is the gap spacing, and \( w \) is the width of the insulating strip. The correction term can be written approximately as

\[ \frac{\Delta C}{C} = \frac{w}{r} \frac{d}{d+0.22w}. \] (A-2)

Typical values of the cell parameters are: \( r = 4 \) mm, \( w = 0.03 \) mm, and \( d = 0.025 \) mm. Using these values one gets for the correction term \( \Delta C/C = 6 \times 10^{-3} \). The simpler expression

\[ C = \frac{\varepsilon \pi r^2}{4d} \text{ (esu)} = \frac{\varepsilon \pi r^2}{d} \text{ (mks)} \] (A-3)
can be used to calculate the capacitance to better than 1% accuracy.

From Eq. (A-3) and using the values of the parameters listed above, the capacitance is \( C = 16 \text{ cm} = 17.8 \text{ pF} \) (1 pF = 0.897 esu·cm). The dielectric constant is set equal to 1 in esu or to 0.0885 pF/cm (\( \varepsilon_0 \)) in mks units. The data are taken with the sample either under vacuum or a few mm of Hg pressure of He gas, thus \( \varepsilon = 1 \) esu. The change in capacitance with a change in gap spacing is given by \( \Delta C / \Delta d = \varepsilon_0 \pi r^2 / d^2 \) = \( C / d \) and is equal to \( 7.1 \times 10^{-5} \text{ pF/Å} \) using the parameters above.

A schematic representation of the electrical circuitry used is shown in Fig. A2. A PAR HR-8 lock-in amplifier provides a reference signal to drive a Bogen power amplifier. The output of the power amplifier is applied to the generator terminals of the GR 1615A capacitance bridge. The capacitance bridge forms the central working component of the electronics. The lock-in is used as the detector for the bridge. The output of the lock-in is displayed on the y-axis of a HP 7000A x-y recorder and the defined "y" axis of a HP data acquisition system. Provision is also included to filter the output of the lock-in before it is displayed on the recorder.

The signal displayed on the x-axis of the recorder comes from the current shunt of the power supply which drives the superconducting solenoid. Provision is made for a Keithley nanovoltmeter to amplify the shunt signal before it goes to the recorder or before it goes to the "x" axis of the acquisition system. A K-5 potentiometer is available for preci-
Fig. A2. Schematic of electrical circuitry for measuring magnetostriction.
sion measurements of the shunt voltage. An ultra low frequency oscillator is used to gate the data acquisition system.

The accuracy of the capacitance bridge is based on the accuracy with which a ratio transformer can be wound. The limit of resolution of the bridge is 1 part in 10^6. At least another order of magnitude in resolution is gained from being able to read the x-y recorder to better than 1 part in 10.

The ultimate electronic resolution of the system for measuring the length change of a sample, which is the negative of the change in the gap spacing, is given by

\[-\Delta L = \Delta d = (\Delta C/C)d = 10^{-7}(0.002) = 0.02 \text{ Å} \quad (A-4)\]

Two types of probes were used in the measurement of the magnetostriction. In both of these probes the electrical leads from the capacitance cell were shielded from each other going to the top of the probe. This was accomplished by running the lead from the top plate of the capacitor through a stainless steel tube and braided shield to a bnc connector at the top of the probe. This is done to minimize parasitic capacitance in parallel with that of the capacitance cell. The only effect of the resulting capacitance to ground is slight degrading of the sensitivity of the detector.

In the longitudinal probe the strain is measured parallel to the direction of the applied field. The alignment of the sample in this probe is estimated to be within 1° of being parallel to the applied field.
The second probe, a transverse probe, allows for measurement of the strain perpendicular to the applied field. The orientation of a known symmetry direction in the sample relative to the field direction can be changed. A spur gear, machined such that a magnetostriction cell slides into it, is mounted to roll on two wheels with a third idler wheel pressing on the top of the spur gear for alignment. The gear has been beveled and runs in grooved wheels. A spiral gear driven through a turns counter at the top of the probe drives the spur gear. The particular spur gear used has 60 teeth so that one turn of the spiral gear rotates the magnetostriction cell 6 degrees. The total angular rotation possible is at least 210°. This is ultimately limited by the heater and carbon resistor thermometer leads which are cemented to the spur gear.

The wobble of the transverse probe about its rotation axis was measured by reflecting a laser beam from the top plate of a cell mounted in position in the gear. The wobble was found to be less than 1°. The average rotation axis of the transverse probe is less than 1/2° from the perpendicular to the field of the solenoid.

2. Magnetization

The magnetization data were taken using the low frequency field modulation technique described by Stark and Windmiller. A low frequency modulation field is used to get uniform penetration of the modulation field into the
sample, i. e. penetration depth much larger than the maximum dimension of the sample. Detection was at the fundamental frequency. This apparatus includes a calibration coil located inside one of the "bucking" coils. It is of the same size and shape as the sample. A schematic drawing of the modulation coil arrangement is shown in Fig. A3. In the construction of the modulation probe, allowance is made so that the coil end of the probe can be rotated ±2° from parallelism to the field in two perpendicular planes.

The susceptibility is measured in the following manner. The reference signal of the lock-in is amplified by the Bogen amplifier and applied to the modulation coils. The phase of the lock-in is set to give "0" signal out when looking at the voltage on the empty "bucking" coil. Then by switching the phase 90° and switching to the difference signal between the "sample" coil and the "bucking" coil, only the signal due to the change in the magnetization of the sample with respect to changes in the applied magnetic field will be observed. The setting of the phase is accomplished at high fields to allow for magnetoresistance of the pick-up coils and to insure penetration of the modulating field due to the sample magnetoresistance. The sample and bucking coils are wired in series opposition and cancel to 1 part in $10^4$.

In the magnetization studies the field was swept so that $(1/H)$ was proportional to time. The signals which are periodic in the reciprocal of the field are now periodic in time, thus allowing real time filtering of the signal. This
Fig. A3. Schematic representation of modulation probe.
is to be contrasted to sweeping $H$ proportional to time in the magnetostriction studies which complicated the analysis of the oscillatory part.

3. Calibration of x-y recorder

**Y axis** The calibration of the $y$-axis for magnetostriction is straightforward. From the equation for strain, $\varepsilon = \Delta L / L_0$, where $L_0$ is the zero field length of the sample and $\Delta L$ is the change in the length which is the negative of the gap change, and using Eq. (A-3) for $d$ one obtains

$$\varepsilon = -\Delta d / L_0 = (1/L_0)(\varepsilon_o A/C^2)\Delta C. \quad (A-5)$$

In Eq. (A-5), $\varepsilon$ is the strain, $\varepsilon_o$ is the dielectric constant, $A$ is the area of the top plate of the capacitance cell, $C$ is the measured capacitance at zero field, and $\Delta C$ is a known change in the setting of the capacitance bridge, say $10^{-4}$ pF, to give some change on the x-y recorder. The length of the sample, $L_0$, was corrected to 4.2 K using the thermal expansion data of McCammon and White.\textsuperscript{39} The area of the top plate was not corrected to 4.2 K but could have been with the information given in Ref. 40. The correction in the area is 7 parts per 1000 which is less than the accuracy of measuring the area. The deflection observed on the x-y recorder then calibrates the $y$ axis in units of strain per inch or per volt.

The calibration of the magnetization is accomplished through the use of a current carrying coil to generate a
known total magnetic moment. The induced voltage in the calibration coil from the modulation field drives a current through an external capacitance which in turn creates an induced magnetic moment in the coil. The equations governing these effects are:

\[ H = H_0 \cos(\omega t) \] 
\[ V = 10^{-8} N A \omega H_0 \sin(\omega t) \] 
\[ I = V(r + i[\omega L - 1/\omega C])^{-1} \] 
\[ = -10^{-8} N A C_0 \omega \sin(\omega t)(\omega) \] 
\[ ([\omega C]^{-1} >> r, \omega L) \] 
\[ \text{Total magnetic moment: } (vM) = NIA/10. \]

The susceptibility is then given by

\[ \frac{d(vM)}{dH} = -10^{-9} (NA\omega)^2 C. \text{ (emu)} \] 

The calibration procedure is completed by comparing the signal due to the calibration coil with that due to the sample,

\[ V_s = 10^{-8} a N_o A_o \frac{d(vM)_{\text{sample}}}{dH} \omega H_0 \] 

where \( N_o \) and \( A_o \) are the number of turns and mean area of the pick-up coil, and \( a \) is a structure factor relating magnetic induction of the sample to the magnetization and the fractional flux linkage with the pick-up coil. The signal observed
when the calibration coil is connected is

\[ V_c = 10^{-8} a N_o A_o \frac{d(vM)_{\text{coil}}}{dH} \omega_{H_o}. \]  

(A-12)

It is important that the external flux of both the sample and
the calibration coil have the same efficiency factor \( a \). In
this case,

\[ \frac{dM_s}{dH} = \frac{dM_c}{dH} \left[ \frac{V_s}{V_c} \right] = 10^{-9} (N A \omega)^2 C \left[ \frac{V_s}{V_c} \right]. \]  

(A-13)

This then calibrates the susceptibility in terms of known
constants and the voltage observed from the calibration coil.

**X axis** The quantity plotted on the x-axis is the volt-
age across the shunt resistor in the power supply. The
current thru this shunt is directly proportional to the mag-
etic field, hence the voltage on the shunt is proportional
to the magnetic field. The calibration of the x-axis was
done by observation of the dHvA effect in beryllium. Using
the known value of the period for the dominant cigar oscil-
lations\textsuperscript{23} allows one to find the constant relating the field
value to shunt voltage. This gave a value of 1.6201 kG/mv
as opposed to the value supplied by the manufacture of
1.59817 kG/mv (70 kG/43.8 mv).
B. Sample Preparation

1) Magnetostriction samples. A Laue oriented boule was spark cut to a length of about 1 cm. The two cut faces are parallel to each other and perpendicular to the principal symmetry direction chosen in the x-ray orientation. The slab is mounted on a post which has a 15° indexing ability, the direction normal to the parallel faces being vertical. The sample is then cut into a square with sides of approximately 9 mm. Using the indexing feature, the corners are cut off at 15° intervals resulting in a sample which is closely the included right circular cylinder of the 9x9x10 mm³ rectangular piece.

2) Magnetization samples. Magnetization samples were cut to a size of 2x3x6 mm³. The 3x6 mm² face defines a known plane in the crystal, while the 6 mm direction of the sample is a known crystal direction within that plane. Samples cut this way may be mounted in the magnetization probe with the known plane aligned with the plane of rotation of the probe.

3) Mounting of the samples. The magnetization samples mount very simply into a nylon holder which slides into the bottom of the magnetization probe. The sample is held in place with vacuum grease.

The magnetostriction sample is soldered to the bottom plate of the magnetostriction cell using In-Cd solder. The solder joint is over the total contact area between the sample and the bottom plate electrode. The cell body is attached
with 3 00-90 screws and the free end of the sample and cell body are simultaneously spark machined to create a coplanar surface. After scribing the cell body and bottom plate of the cell, the cell body is removed and the length of the sample is measured. Once this is accomplished, the cell body is replaced in its previous position, the mylar washer used as the spacer is placed on the top of the cell body, and the top plate is secured with 3 00-90 screws. If no shorts are found, the magnetostriction cell is ready for use.
C. Fourier Transforms of Simple Cases

Consider a function \( Y = f(X) \) defined between \( X = X_1 \) and \( X = X_2 \). The Fourier Transform of such a function is given by

\[
G(\omega) = \int_{-\infty}^{\infty} Y e^{i\omega X} dX = \int_{X_1}^{X_2} f(X) e^{i\omega X} dX. \tag{C-1}
\]

Now transform to a symmetric interval such that \( Y = g(X') = f(X + X_0) \) and defined between the limits of \( \pm L/2 \) where

\[
L = X_2 - X_1 \\
X_0 = (X_1 + X_2)/2. \tag{C-2}
\]

Then \( G(\omega) \) becomes

\[
G(\omega) = \int_{-L/2}^{L/2} f(X + X_0) \exp(i\omega [X + X_0]) dX. \tag{C-3}
\]

Now take \( Y = A \cos(\omega_0 X + \phi) \). For this function the transform is given as

\[
G(\omega) = A \int_{-L/2}^{L/2} \cos(\omega_0 [X + X_0] + \phi) \exp(i\omega [X + X_0]) dX \\
= A \exp(i[\omega_0 + \omega]X_0 + \phi) \frac{\sin([\omega_0 + \omega]L/2)}{\omega_0 + \omega} \\
+ A \exp(-i[\omega_0 + \omega]X_0 + \phi) \frac{\sin([\omega_0 - \omega]L/2)}{\omega_0 - \omega}. \tag{C-4}
\]

At \( \omega = \omega_0 \), the first term will be of order \( A/2\omega_0 \) whereas the second term will be of order \( AL/2 \). Neglect of the term in \( (\omega_0 + \omega) \) will have little effect on the transform for large positive \( \omega \)'s. Then to a good approximation
\[ G_1(\omega) = A \exp(-i[\omega_o - \omega]X_0 + \phi]) \frac{\sin([\omega_o - \omega]L/2)}{\omega_o - \omega}. \]  \hspace{1cm} (C-5)

The amplitude of \( G_1 \) as a function of \( \omega \) is peaked at \( \omega = \omega_o \) dropping off on either side as \( (\omega_o - \omega)^{-1} \) with zero values for the argument of the sine term equal \( n\pi \). The magnitude of the power spectrum of the transform at \( \omega = \omega_o \) is given by

\[ |G_1(\omega_o)| = AL/2. \]  \hspace{1cm} (C-6)

Zeros of \( G_1 \) occur at \( (\omega_o - \omega)L/2 = \pm n\pi \) for \( n = 1, 2, 3, \ldots \).

Consider a damped cosine function defined between \( X_1 \) and \( X_2 \):

\[ Y = A \exp(-\alpha X) \cos(\omega_o X + \phi). \]  \hspace{1cm} (C-7)

The Fourier Transform of this function by Eq. (C-3) is

\[ G_2(\omega) = A \int_{-L/2}^{L/2} \cos(\omega_o [X+X_o] + \phi) \exp((i\omega - \omega_o) [X+X_o]) dX 
= A \exp(-i[\omega_o - i\alpha]X_o + \phi]) \]
\[ \times \frac{\sinh(i[\omega_o - \omega_o]L/2)}{i(\omega_o - \omega) + \alpha}. \]  \hspace{1cm} (C-8)

This is a function whose amplitude is peaked at \( \omega = \omega_o \) and drops off on either side of the central peak again as \( (\omega_o - \omega)^{-1} \). The term in \( (\omega_o + \omega) \) has been dropped as before. The amplitude of the power spectrum at \( \omega = \omega_o \) is given by

\[ |G_2(\omega = \omega_o)| = A \exp(-\alpha X_o) \sinh(\alpha L/2)/\alpha. \]  \hspace{1cm} (C-9)

Consider the magnitude of \( G_2 \) at the zeroes of \( G_1 \), \( \omega_o - \omega = 2n\pi/L \),
From these last two equations, two equations in two unknowns can be written. The damping, \( \alpha \), can be found by taking

\[
\left| G_2(\omega_0 - \omega = 2n\pi/L) \right| / \left| G_2(\omega = \omega_0) \right|^2 \quad \text{for } n=1 \quad \text{(corresponding to the first zero point on either side of the central peak)}. \]

This gives

\[
R = \alpha^2 / \left( [2\pi/L]^2 + \alpha^2 \right). \quad \text{(C-11)}
\]

Solving this expression for the damping gives

\[
\alpha = (2\pi/L) \left[ R/(1-R) \right]^{1/2}, \quad \text{(C-12)}
\]

where only the positive root is considered as \( \alpha \) is assumed to be positive only. Substituting this value for \( \alpha \) into Eq. (C-9), the value of the amplitude, \( A \), can be found.

If the numerical transform of a function such as one given by Eq. (C-7) was available it should be possible to find these two parameters, \( \alpha \) and \( A \). The phase, \( \phi \), can be found from the arctangent of the imaginary part of \( G_2 \) divided by the real part of \( G_2 \) for \( \omega = \omega_0 \).

Some trial programs were written to calculate the Fourier Transform as given by Eq. (C-8). Data were then generated with parameters \( \omega_0 \), \( \alpha \), \( \phi \), and \( A \). This data was analyzed using a routine similar to TRANS as described in Appendix E.
It was found that if the generated data had at least 5 points per cycle, the transform routine found the proper frequencies. However, to be able to use the above described technique to find the amplitude and damping factors, it was determined that at least 20 points per cycle must be present in the data. Even at this level the calculated transform gave an amplitude at the center frequency of only 90% of that calculated by Eq. (C-8).

For data with one frequency component, the above procedure gave reliable results. With two or more components in the data separated by at least 10% from each other the results were still acceptable. When the data had more than one term separated less than 10-15%, the above procedure failed to work. The reason for this is the cross terms generated in the power spectrum of the Fourier Transform. The contribution from each frequency component to the value of the Fourier Transform at a particular frequency can be an appreciable fraction of the total magnitude of the transform when there are several terms close together.
D. Non Linear Least Squares

The linear least squares fitting of data to a polynomial expansion is well known. Let us apply linear least squares fitting to a non linear function. Consider a function given by

\[ Y = \sum A_i e^{-\alpha_i x} \cos(\omega_i x + \phi_i). \]  

(D-1)

Making use of the slowly varying nature of the exponential function, approximate \( Y \) for a small range of \( x \) as

\[ Y = \sum B_i \cos(\omega_i x + \phi_i) \]  

(D-2)

where \( B_i \) is the average value of \( A_i e^{-\alpha_i x} \) for a small range of \( x \). Now \( Y \) may be expanded as

\[ Y = \sum B_i [\cos(\omega_i x) \cos \phi_i - \sin(\omega_i x) \sin \phi_i] \]

\[ = \sum [a_i \cos(\omega_i x) + b_i \sin(\omega_i x)] \]  

(D-3)

where

\[ a_i = B_i \cos \phi_i \]
\[ b_i = B_i \sin \phi_i \]  

(D-4)

which inverted gives

\[ B_i = [a_i^2 + b_i^2]^{1/2} \]
\[ \phi_i = \tan^{-1}[-b_i/a_i]. \]  

(D-5)

Using Eq. (D-3) with the \( \omega_i \)'s assumed known and constant perform a least squares fitting to find the a's and b's.
This will involve minimizing the sum of the squares of the deviations, i.e. minimizing the function

$$\sum_j [Y_j - \sum_i (a_i \cos(\omega_i X_j) + b_i \sin(\omega_i X_j))] = \Sigma d^2$$  \hspace{1cm} (D-6)

with respect to $a_i$'s and $b_i$'s holding the $\omega_i$'s constant. Thus one needs

$$\frac{\partial (\Sigma d^2)}{\partial a_k} = 0$$

$$\frac{\partial (\Sigma d^2)}{\partial b_k} = 0$$  \hspace{1cm} (D-7)

where $k$ runs over the same range as $i$ (1-M) for the $j$ (1-N) data points. Doing these derivatives gives

$$\sum_j \sum_i [a_i \cos(\omega_i X_j) + b_i \sin(\omega_i X_j)] \cos(\omega_k X_j) = \sum_j Y_j \cos(\omega_k X_j)$$

$$\sum_j \sum_i [a_i \cos(\omega_i X_j) + b_i \sin(\omega_i X_j)] \sin(\omega_k X_j) = \sum_j Y_j \sin(\omega_k X_j).$$  \hspace{1cm} (D-8)

This equation might be stated formally as: Write down Eq. (D-3) for each data point, multiply each of these equations by the coefficient of $a_1$ and sum the resulting equations. Repeat this for $a_2$, $a_3$, ..., $b_M$. The normal equations, Eq. (D-8) is a matrix equation $AX=B$ which is to be solved for $X$ using any convenient means. Once the $X$ (a$_i$'s and b$_i$'s) is known, the B$_i$'s and $\phi_i$'s of Eq. (D-5) may be determined. Repeating this procedure using different ranges of a total data span, a vector of values of $X$ at the center of a small range (window) along with the values obtained for a particular
$B_i$ can be formed. By fitting the $\ln(B)$ to a straight line, an approximation for the $A_i$ and the $\alpha_i$ in Eq. (D-1) may be determined.

A routine using this procedure was written. It was found that for one term in Eq. (D-1), ($M=1$), this procedure determines the parameters accurately with about 6 points per cycle present in the data. It was learned, as is shown by information theory, that for more than one term in the data, the range of $X$ (window) that is used to find the $a$'s and $b$'s must contain at least one cycle of the smallest difference frequency present in the data.
E. Computer Program Used in Analysis

1. Description of program

Included in this appendix is a discussion of the program used, a definition of the input variables, and a listing of the program.

MAIN The mainline is used to initiate the program and contains most of the storage allocations. The plot routine is started and stopped in the mainline. (The plot routine used is particular to the system and will probably need major modifications for other systems.) The calls to SETX, SETY, and SETI are used to initialize the plot page parameters. Plot page parameters can be changed at any time by appropriate calls to the proper subroutine. The program automatically repeats for as many data sets as desired.

SINCOS sets up a table of $\sin \theta$ and $\cos \theta$ for 1000 values of the argument, $\theta$, between 0 and 0.999(2$\pi$) using the library functions in the computer. This table is calculated only once each time the program is run.

READER reads in two numbers (NX, NH) which are used to tell the routine the form of the data. All other parameters for the current data set are then read. The data set may have been recorded on paper tape in which case it is necessary to average over the X's (H values) as the readings for X and Y are not simultaneous but are ordered in time. The difference in NX and NH tell how many points to average. If these two parameters are equal the values for H are calculated
in this routine. The resulting data can be plotted to see if it agrees with the x-y recorder tracing. For NX less than NH the data is read in as ordered pairs of (H,YH).

The routine scales the data into physical units, orders the data increasing (H increasing) and culls out the data for H less than 3 kG. If in this routine, no more data can be found, IFIN is set equal to 1 which stops the program.

FIT is used to prepare the data for a least squares fit to determine the parameters describing the monotonic part of the data. In order, this routine sets up the data for the entire range of the data, for the low field portion through HFLOW, and for the high field portion above HFHIGH. Provision is made through the parameter ISWEEP to skip either the low field or high field portion of the analysis if the data set does not contain one of these regions. A plot routine is included to plot $\gamma/H^2$ for the data, the high field fit, the low field fit, and the total field fit on one plot page.

The analysis of a data set is terminated if at any time in the solution of the monotonic portion the parameter KS from SIMQ is set equal to 1. The routine SIMQ is a library function for the solution of the matrix equation $AX=B$ and $KS=1$ says $\det(A)=0$.

**BASLIN** This routine finds a vector, (CAPH, CAPYH), which is some type of average representation of the data. A polynomial expansion in $\text{CAPH}^2$ is done to this vector using the subroutine LSTSQU.
The different averaging options included in this routine are: The vector \((\text{CAPH}, \text{CAPYH})\) can be made up of all the data points, of the average of a minimum and maximum of the extremals for oscillatory data, or of averages of \(H\) and \(YH\) in the width of data, \(\text{WINDOW}\), stepped through the data by \(\text{WNDSTP}\). If the parameter \(\text{IBASE}\) is 0 the expansion coefficients are defined to be zero, i.e. no baseline is to be found or subtracted from the data.

The vector \((\text{CAPH}, \text{CAPYH})\) is changed into \((\text{CAPH}^2, \text{CAPYH})\) and for \(\text{JUMP}=0\), which is for the high field portion of the data to have no constant term, into \((\text{CAPH}^2, \text{CAPYH}/\text{CAPH}^2)\). This vector is fit to a polynomial using a least squares method. The baseline is calculated from the coefficients found by \(\text{LSTSQU}\). A provision is made to plot the raw data and the calculated data on the same page through the parameter \(\text{NPLTDT}\).

\(\text{SOLA}\) subtracts the baseline representation of the high field portion of the data, multiples the data by the proper power of \(H\) to transform it into a damped sinusoid form, inverts the \(H\) values to give \(1/H\), and properly reorders \(1/H\), \((H)\), and \(Y(1/H)\), \((YH)\). The Fourier Transform of the data is done thru \(\text{TRANS}\) for the frequency range \(\text{OMEGAL}-\text{OMEGAU}\) in steps of \(\text{DOMEGA}\).

The routine executes two different methods for finding the damping, \(\text{ALPHA}\), and the amplitude, \(\text{AMPLIT}\) or \(\text{AMP}\), for \(\text{IMPOSE}\) terms in the data. This first method is based on the discussion presented in Appendix C. The second method uses
a linear least squares fit to a non-linear function as discussed in Appendix D.

In this second method a window width, HIWIN, and a step size, HIINC are defined. The window width is set equal to 5 times the period (contains five cycles of data) if there is to be only one term analyzed (IMPOSE=1). For more than one term to be analyzed (IMPOSE>1), HIWIN is set equal to 0.8 times the longest period difference of the IMPOSE frequencies. A fit as described in Appendix D is done to find the representation for the amplitude in a window. The window is moved by HIINC and the analysis repeated. This is done for the entire range of the data. The vector formed from the logarithm of the amplitude and the center 1/H of a window is fit to a straight line, the intercept giving the amplitude and the slope gives the damping for the relevant frequency term. This is repeated for each frequency term claimed to be present in the data, IMPOSE.

The next data card is read and if it contains a non-zero DOMEGA, this subroutine is repeated.

TRANS calculates the real and imaginary parts of the Fourier Transform of the data. This transform is performed for the frequency range F to FREQU in steps of DFREQ. These are renamed variables for programming convenience. The arguments of the sine and cosine terms involved are products like 2\pi fX. Dividing the argument by 2\pi and retaining the decimal portion reduces the argument to its principal value. The decimal portion is multiplied by 1000. This result plus 1 is
used as the subscript to look up the values for sines and
cosines as calculated in SINCOS. Thus to save a step in the
calculations only the product fX is calculated. No visible
change in accuracy was noticed using this method for cal­cu-
lating the sines and cosines. A simple trapezoidal summing
is done for the integration.

MINMAX finds the extremums in the set (X,Y). This is
accomplished by comparing $Y_i$ to $Y_{i-1}$ and seeing if $Y_i$ is
larger (a minimum) or smaller (a maximum) than $Y_{i-1}$. For
non-equally spaced data, this routine will only return values
of data in the extremum vectors. The variable IFIT must be
set equal to 0 in the call to MINMAX. For data equally
spaced in X, there is a provision to fit the extremum points,
i-1, i, i+1, to a quadratic and from this find the calcula-
ted extremum.

LSTSQU is a linear least squares fit to a polynomial of
degree M with N data points. This subroutine also calculates
estimates of the variation of the coefficients. The routine
SIMQ is a library function for solving the matrix equation
$AX=B$.

DETER calculates the determinant of a square matrix
using the pivotal method on the largest element in a column.

YGRAPH along with SET and EXTRMA are used to plot a
vector, $(X, Y)$ off-line on a Calcomp plotter. In YGRAPH
 provision is made to plot one curve per plot page or to plot
as many curves as desired on one plot page, all with the
same plot page parameters.
SET is used to set the length and margins for the X and Y axis and to set the center symbol, (ISYM), to be placed at each plotted point.

EXTRMA finds the minimum and maximum values for the "B" axis, the value of the variable at the origin of the plot page, and the spacing of the tick marks appearing on the plot page. All of these values are calculated as a multiple of some power of ten. The functions AINT, SIGN, AMAX1, and AMIN1 are library functions.

Following is a description of the input parameters and a listing of the program.
2. Definition of symbols and program listing

NX  Number of raw data points if data is from paper
tape, otherwise is a dummy number used for control
in READER.

NH  Number of data points - pairs of \( (H, Y_H) \), beforeing
culling for \( H \) less than 3 kilogauss.

NPLTDT  0 - Do; 1 - Do not plot data and fitted function,
i.e. \( Y \) vs \( H \) in subroutine BASLIN.

NOPLOT  0 - Do; 1 - Do not plot \( (Y-Y_0)_\text{data}/H^2 \) and fitted
functions in form \( (Y-Y_0)_\text{fit}/H^2 \) in subroutine FIT.

NPLTHI  0 - Do; 1 - Do not plot \( Y(1/H) \) vs \( 1/H \) in SOLA.

NPLTPS  0 - Do; 1 - Do not plot power spectrum in SOLA.

NTRANS  0 - Do; 1 - Do not execute SOLA.

IBASE  0 - Define expansion parameters for baseline as 0.
1 - Do window routine which averages data to remove
oscillatory data.

2 - Take average of maximum and minimum of oscil-
latory data to find baseline.

3 - Take all of the data points to find baseline.

MORDER  Order of polynomial for baseline fit for high and
total expansions. Low field is defined as quadratic.

MAG  0 - Data set is magnetostriction data. After sub-
tracting baseline multiply result by \( H^{1/2} \).

1 - Data set is magnetization data. After sub-
tracting baseline multiply result by \( H^{5/2} \).

IDENT  Data set identification number, 1-6 digit number.
ISWEEP Used in magnetostriction analysis to specify if data set is FULL, LOW, or HIGH sweep. These words are the possible values for this variable.

YO Zero adjustment for strain data to make Y=0 at H=0.

HSUP Voltage corresponding to H=0 magnetic field.

HSSCALE Scaling constant to convert H(volts) to H(kG).

HFLOW Maximum field range for low field expansion in data.

HHIGH Minimum field range for high field expansion region.

YSCLAL Yscale factor to convert Y(volts) to Y(physical units). This variable is YSCALE upon exit from subroutine READER.

DEOMEGA Sets the size of the frequency increment for Fourier Transform. Read in as increment in number of cycles, program converts it into frequency (kG). This variable and the difference of the next two determine how many frequency terms are to be calculated in Fourier Transform, limited to 400.

OMEGAL Lowest frequency for Fourier Transform. Read in as minimum number of cycles expected in sweep range and converted to frequency (kG) in program.

OMEGAU Highest frequency for Fourier Transform. Read in as maximum number of cycles expected in sweep range and converted to frequency (kG) in program.

The next 10 variables are used only when the H values are to be generated by the program. Included in this portion of READER is provision to plot this calculated data for comparison with the x-y recorder tracing.
HMIN  Minimum value of H for the data set.
HMAX  Maximum value of H for the data set.
XMIN  Voltage value on left side of recorder page, will be the value for left side of plot page.
XMAX  Voltage value on right side of recorder page, will be the value for right side of plot page.
INCR  Tells whether the data was recorded with H increasing (=1) or decreasing (=0).
N     Number of data set points, set equal to NH
IDENT Same as above, must be on card at all times.
XLENG Sets the length of the plot page in inches. Equal to the length of the x-y recorder page between XMIN and XMAX plus 2 inches.
NPLT  0 - Do; 1 - Do not plot the generated data.
IHO10H 0 - H swept linear in time; 1 - 1/H swept linear in time.
X     Raw data, H values.
IX    Exponent read in to convert X into volts due to characteristics of acquisition system.
YX    Y values corresponding to X raw data.
IYX   Exponent used to convert YX into volts.

NOTES: 1. The vector (X, YX) is changed into (H, YH).
        2. The variables H and YH are renamed and reordered in SOLA to HI and YHI to conserve storage.
        3. If there is only one frequency range to be analyzed for a data set, there must be a blank card as the last card in the data set.
4. When a data set has more than one frequency range to be analyzed an appropriate number of cards with the parameters for the Fourier Transform are affixed to the end of the data set. A blank card is always the last card in a data set deck.

A listing of the program follows.
MAINLINE

COMMON/A/SINFT(1000),COSFT(1000)
COMMON/B/H(2500),YH(2500),NH
COMMON/C/OMEGA(450),RFT(450),UFT(450),PWR(450),NFT
COMMON/D/NPLTHI,NPLTPS,NTRANS
COMMON/E/NPLTDT,IBASE,MORDER,NOPLOT,YO
COMMON/F/DOMEGA,OMEGAL,OMEGAU,IMPOSE
COMMON/G/B(10),C(10),SUMDIF,SIGMA
COMMON/H/YSCALE,IDENT,ISWEEP,HFLOW,HFHIGH,MAG

SET UP GENERAL PLOT PAGE PARAMETERS

CALL PENPOS('CARTER, JAMES',13,1)
CALL SETY(11.0,0.5)
CALL SETX(17.0,1.0)
CALL SETI(-1)
CALL SINCOS

NOW BEGIN DATA ANALYSIS

CALL READER(IFIN)
IF(IFIN.EQ.1) GO TO 9999
CALL FIT(KS)
IF(KS.EQ.0) GO TO 20
15 READ(1,1006) DOMEGA
IF(DOMEGA.GT.0.0) GO TO 15
WRITE(3,1007) Go TO 10
20 IF(NTRANS.EQ.0) CALL SOLA
WRITE(3,1008) IDENT,ISWEEP,YSCALE
GO TO 10
1006 FORMAT(F10.3)
1007 FORMAT('O ***SINGULAR MATRIX ENCOUNTERED***',
1 1X,'TERMINATE THIS DATA SET - BEGIN NEXT')
1008 FORMAT(///,10X,'THIS COMPLETES THE ANALYSIS OF',
1 1X,'RUN NUMBER',15,'WHICH WAS A ',A4,' FIELD',
2 1X,'SWEEP; WITH YSCALE =',E18.8)
9999 CONTINUE
CALL LSTPLT
STOP
END

SUBROUTINE SINCOS

PURPOSE

CALCULATE SIN AND COSINE TABLES
1000 VALUES OF ARG - 0.0 TO 2 PI
SUBROUTINE READER(IFIN)

C PURPOSE
C
READ IN DATA, SCALE DATA, AND ORDER DATA
ALSO CULL OUT DATA FOR H<3.0 KILOGAUSS
WRITE OUT INPUT PARAMETERS

C USAGE: CALL READER(IFIN)

C DESCRIPTION OF PARAMETER: IFIN=1 MEANS NO MORE DATA

COMMON/B/H(2500),YH(2500),NH
COMMON/D/NPLTHI,NPLTPS,NTRANS
COMMON/E/NPLDTI,IBASE,MORDER,NPLOT,Y0
COMMON/F/DOMEGA,OMEGAL,OMEGAU,IMPOSE
COMMON/H/YSCAL,IDENT,ISWEEP,HFLOW,HFHigh,MAG
COMMON/WK1/X(2500),IX(2500),YX(2500),IYX(2500)

IF(IFIN=0)

10 READ(1,1000,END=9999)NX,NH
READ(1,1001)NPLTDT,NPLOT,NPLTHI,NPLTPS,NTRANS,
IBASE,MORDER,MAG,IDENT,ISWEEP,Y0,HSup,HSCALe,HFLOW,
2HFHigh,YSCAL,DOMEGA,OMEGAUM,OMEGAU,IMPOSE
WRITE(3,1002)IDENT,ISWEEP,HSCALe,YSCAL,HSup,Y0,
1HFLOW,HFHigh,IBASE,MORDER
READ(1,1003)HMIN,HMAX,XMIN,XMAX,INCR,N,IDENT,XLENG,
1NPLT,TH010H
IF(NX.LT.NH)GO TO 50
IF(NX.EQ.NH)GO TO 55
IA=NX-NH+1
READ(1,1004) (X(J),IX(J),YX(J),IYX(J),J=1,NX)
C
SCALE X AND YX INTO VOLTS
C
DO 15 I=1,NX
   X(I)=X(I)/10.0**IX(I)
   YX(I)=YX(I)/10.0**IYX(I)
15 CONTINUE
WRITE(3,1005)(X(J),YX(J),J=1,NX)
C
TIME AVERAGE THE DATA TO REMOVE NOISE IN X
C
DO 15 I=1,NX
   X(I)=X(I)/10.0**IX(I)
   YX(I)=YX(I)/10.0**IYX(I)
15 CONTINUE
WRITE(3,1005)(X(J),YX(J),J=1,NX)
C
HAND READ DATA
C
READ(1,1006) (H(J),YH(J),J=1,NH) GO TO 95
C
CALCULATE H FOR LINEAR SWEET IN H
C
IF(IO1OH.EQ.1) GO TO 75
   DELH=(HMAM-HMIN)/(N-1)
   READ(1,1007) (YX(I),IYX(I),I=1,N)
   IF(INCR.EQ.1) GO TO 65
   DO 60 I=1,N
      K=N-I+1
      H(K)=HMAM-DELH*(I-1)
      YH(K)=YX(I)/10.0**IYX(I)
60 CONTINUE
GO TO 90
65 DO 70 I=1,N
   H(I)=HMIN+DELH*(I-1)
   YH(I)=YX(I)/10.0**IYX(I)
70 CONTINUE
   GO TO 90

       CALCULATE H FOR LINEAR SWEEP IN 1/H

75   DEL10H=(1.0/HMIN-1.0/HMAX)/(N-1)
   READ(1,1007) (YX(I),IYX(I),I=1,N)
   IF(INCR.EQ.1) GO TO 83
   DO 80 I=1,N
      K=N-I+1
      H(K)=1.0/(1.0/HMAX+DEL10H*(I-1))
      YH(K)=YX(I)/10.0**IYX(I)
80 CONTINUE
   GO TO 90
83   DO 85 I=1,N
      H(I)=1.0/(1.0/HMIN-DEL10H*(I-1))
      YH(I)=YX(I)/10.0**IYX(I)
85 CONTINUE
90 IF(NPLT.EQ.1) GO TO 95
   CALL NEWPLT(1.0,5.5,XLENG)
   CALL ORIGIN(XMIN,0.0)
   CALL XSCALE(XMIN,XMAX,XLENG-2.0)
   CALL YSCALE(-10.0,10.0,10.0)
   CALL XAXIS((XMAX-XMIN)/(XLENG-2.0))
   CALL YAXIS(1.0)
   CALL XYPLT(H,YH,N,1,-1)
   CALL ENDPLT

       PUT DATA IN ASCENDING ORDER AND SCALE H

95 IF(H(NH).GT.H(1)) GO TO 105
   NO2=NH/2
   DO 100 I=1,NO2
      K=NH-I+1
      HK=H(I)
      H(I)=H(K)*HSCALE
      H(K)=HK*HSCALE
      YHK=YH(I)
      YH(I)=YH(K)
      YH(K)=YHK
100 CONTINUE
   IF((K-I).GT.1) H(I+1)=H(I+1)*HSCALE
   GO TO 115
105 DO 110 I=1,NH
      H(I)=H(I)*HSCALE
110 CONTINUE
C
C CULL H LESS THAN 3.0 KILOGAUSS
C THIS IS DOWN AS SOLENOID IS UNSTABLE IN THIS
C REGION OF FIELD
C
115 CONTINUE
J=0
120 J=J+1
   IF(H(J).LT.3.0) GO TO 120
   DO 125 I=J,NH
      H(I-J+1)=H(I)
      YH(I-J+1)=YH(I)
   125 CONTINUE
   NH=NH-J+1
   WRITE(3,1008) IA,(H(J), YH(J),J=1,NH)
1000 FORMAT(2I5)
1001 FORMAT(8I2,/,I6,A4,5F10.7,E18.8,/,3F10.3,I5)
1002 FORMAT('1' ***** THIS IS RUN NUMBER 'I5, 1'
   ' *****',/,'5X,' WHICH IS A ','A4,' FIELD SWEEP',/,'5X, 2'HSCALER =',F15.7,5X,'Y SCALER =',E18.8,/,5X, 3'H SUPPRESS IN VOLTS =',F15.7,5X,'Y0 IN VOLTS =', 4F10.7,/,5X,'LOW FIELD RANGE <',F10.7,5X, 5'HIGH FIELD RANGE >',F10.7,/,5X,'USE BASE ROUTINE',I3, 6' FOR H**(2*I2,' ) EXPANSION',/)
1003 FORMAT(4F10.4,3I5,F5.0,2I5)
1004 FORMAT(8(2X,F7.0,I1))
1005 FORMAT(/,' THE RAW DATA ARE: ',/,'8(2X,F8.4))
1006 FORMAT(8F10.4)
1007 FORMAT(4(12X,F7.0.I1))
1008 FORMAT(/,' THE AVERAGED DATA OVER ',I3, 1' DATA POINTS ARE: ','/,'8(2X,F8.4))
RETURN
9999 IF(IN=1
RETURN
END

SUBROUTINE FIT(KS)

C
C PURPOSE:
C
C FIX UP DATA TO DO EXPANSION TO BY BASLIN AND PLOT
C
C USAGE: CALL FIT(KS) KS-COND. CODE FROM SIMQ
C
C METHOD
C
C FITS TOTAL RANGE OF DATA TO MORDER POLY. IN H**2
C INCLUDING A CONSTANT TERM; A QUADRATIC EXPANSION
C IN H**2 INCLUDING A CONSTANT TERM IN LOW FIELD
C RANGE (H-HFLOW) AND AN MORDER-1 EXPANSION IN
C H**2 FOR HIGH RANGE OF DATA SET WITHOUT A CONSTANT
H(>HFHIGH).

COMMON/B/H(2500),YH(2500),NH
COMMON/E/NPLDTT,IBASE,MORDER,NOPLOT,YO
COMMON/G/B(10),C(10),SUMDIF,SIGMA
COMMON/H/YSCALE,IDENT,ISWEEP,HFLOW,HFHIGH,MAG
COMMON/WK1/X(2500),Y(2500),XX(2500),YY(2500)
DIMENSION A(3,10),V(3,10),RMSD(3)
INTEGER SWEEP(3) /'FULL'/
INTEGER LOW/'LOW'/,HIGH/'HIGH'/

MP1=MORDER+1
N=NH
DO 5 I=1,NH
  X(I)=H(I)
  Y(I)=YH(I)
5 CONTINUE
CALL SETX(17.0,1.0)
CALL SETY(11.0,0.5)

FULL EXPANSION

CALL BASLIN(KS,1)
IF(KS.EQ.1) GO TO 99
KQ=1
RMSD(KQ)=SIGMA*YSCALE
DO 10 I=1,MP1
  A(KQ,I)=B(I)
  V(KQ,I)=YSCALE*C(I)
10 CONTINUE

LOW FIELD EXPANSION

IF(ISWEEP.EQ.HIGH) GO TO 29
DO 20 I=1,N
  IF(X(I).GT.HFLOW) GO TO 25
  H(I)=X(I)
  YH(I)=Y(I)
20 CONTINUE
25 NH=I-1
MORDER=2
NTL=MORDER+1
CALL BASLIN(KS,1)
KQ=KQ+1
SWEEP(KQ)=LOW
IF(KS.EQ.1) GO TO 99
RMSD(KQ)=SIGMA*YSCALE
DO 28 I=1,NTL
  A(KQ,I)=B(I)
  V(KQ,I)=C(I)*YSCALE
28 CONTINUE

HIGH FIELD EXPANSION
IF(ISWEEP.EQ.LOW) GO TO 40

29 NT=0
 MORDER=MP1-2
 DO 30 J=1,N
 IF(X(J).LT.HFHIGH) GO TO 30
 NT=NT+1
 YH(NT)=Y(J)
 H(NT)=X(J)
30 CONTINUE
 NH=NT
 CALL BASLIN(KS,0)
 KQ=KQ+1
 SWEEP(KQ)=HIGH
 IF(KS.EQ.1) GO TO 99
 RMSD(KQ)=SIGMA*YSCALE
 NT=MORDER+1
 DO 35 I=1,NT
 A(KQ,I)=B(I)
 V(KQ,I)=YSCALE*C(I)
35 CONTINUE

C
C PLOT Y/H**2 VS H**2
C
40 IF(NOPLOT.EQ.1) GO TO 65
 L=0
 KJD=N/100+1
 DO 45 I=1,N,KJD
 L=L+1
 HH=X(I)*X(I)
 XX(L)=HH
 H2=HH
 YY(L)=A(1,2)
 DO 45 J=3,MP1
 YY(L)=YY(L)+HH*A(1,J)
 HH=HH*H2
45 CONTINUE
 CALL SETI(3)
 CALL YGRAPH(XX,YY,L,'FULL',4,2,1)
 IF(ISWEEP.EQ.LOW) GO TO 53
 L=0
 DO 50 I=1,N,KJD
 L=L+1
 HH=XX(L)
 H2=HH
 YY(L)=A(KQ,1)
 DO 50 J=2,NT
 YY(L)=YY(L)+HH*A(KQ,J)
 HH=HH*H2
50 CONTINUE
 CALL SETI(4)
 CALL YGRAPH(XX,YY,L,'HIGH',4,2,2)
 IF(ISWEEP.EQ.HIGH) GO TO 58
53 L=0
HSTOP = 1.44 * HFLOW * HFLOW
DO 55 I = 1, N, KJD
   L = L + 1
   XX(L) = X(I) * X(I)
   HH = XX(L)
   IF (HH .GT. HSTOP) GO TO 57
   YY(L) = A(2, 2) + HH * A(2, 3)
55 CONTINUE
57 CALL SETI(11)
   CALL YGRAPH(XX, YY, L - 1, ' LOW', 4, 2, 3)
58 DO 60 I = 1, N
   XX(I) = X(I) * X(I)
   IF (ISWEEP .EQ. HIGH) YY(I) = Y(I) / XX(I)
   IF (ISWEEP .NE. HIGH) YY(I) = (Y(I) - A(2, 1)) / XX(I)
60 CONTINUE
   CALL SETI(-1)
   CALL YGRAPH(XX, YY, N, 'Y - A/H**2 VS H**2', 16, 1, 99)
C WRITE OUT EXPANSION PARAMETERS
C
65 CONTINUE
   DO 70 I = 1, KQ
       DO 70 J = 1, MP1
           A(I, J) = A(I, J) * YSCALE
70 CONTINUE
   NT = MP1
   DO 75 I = 1, KQ
       IF (I .EQ. 2 .AND. ISWEEP .NE. HIGH) NT = NTL
       IF (I .EQ. KQ .AND. ISWEEP .NE. LOW) NT = MORDER + 1
       WRITE(3, 100) SWEEP(I), X0, (J, A(I, J), V(I, J), J = 1, NT)
75 CONTINUE
   WRITE(3, 101) YSCALE, (SWEEP(I), RMSD(I), I = 1, KQ)
100 FORMAT(//, 10X, 'COEFFICIENTS AND VARIATIONS FOR THE ',
            2(1X, 'A4', ' FIELD EXPANSION WITH Y0 = ', E18.8, ', ARE:', //,
            2(5X, 'A(', I2, ') = ', E18.8, '+/-', E18.8, '/))
101 FORMAT(//, 10X, 'YSCALE FACTOR IS ', E18.8,//, 10X, 'IN UNITS OF STRAIN, THE STANDARD DEVIATION FOR', //,
            2(10X, A4, ' FIELD IS ', E18.8, '/))
99 RETURN
END

SUBROUTINE BASLIN(KS, JUMP)
C PURPOSE: TO FIND EQUATION OF BASELINE OF DATA
C
USAGE: CALL BASLIN(KS, JUMP)
C
DESCRIPTION OF PARAMETERS
C
   KS - CONDITION CODE FROM SIMQ FOR DET=0
METHOD

FIND AVERAGE COORDINATES OF DATA IN A WINDOW 10% OF THE DATA WIDTH. FIND AVERAGE Y, MOVE WINDOW 2%, FIND AVERAGE Y, REPEAT UNTIL RIGHT SIDE OF WINDOW EXCEEDS DATA LIMIT - OR - FIND EXTREMA OF DATA, TAKE AVERAGE OF CONSECUTIVE MINIMUM AND MAXIMUM - OR - TAKE ALL OF DATA POINTS --- FIT THESE AVERAGE X AND Y'S AS AN MORDER POLYNOMIAL IN H**2 USING SUBROUTINE LSTSQU

COMMON/B/H(2500),YH(2500),NH
COMMON/E/NPLDTS,IBASE,MORDER,NOPLOT,Y0
COMMON/G/B(10),C(10,SUMD,SIGMA
COMMON/WK1/S1(2500),S2(2500),CAPH(2500),CAPYH(2500)
COMMON/WK2/H(100),YHL(100),HH(100),YHH(100)

MP1=MORDER+1
IF(IBASE.EQ.0) GO TO 110
IF(IBASE.EQ.2) GO TO 50
IF(IBASE.EQ.3) GO TO 60

WINDOW=(H(NH)-H(1))/10.0
WNDSTP=WINDOW/5.0
10 NUMB=0
HLOW=H(1)
HHIGH=HLOW+WINDOW
ISTART=1
20 NUMB=NUMB+1
K=0
DO 30 I=ISTART,NH
IF(H(I).LT.HLOW) GO TO 30
K=K+1
IF(K.EQ.1) ILOW=I
25 IF(H(I).GT.HHIGH) GO TO 35
30 CONTINUE
35 IHIGH=I-1
IF(IHIGH.GT.ILOW) GO TO 40
WINDOW=2.0*WINDOW
WNDSTP=2.0*WNDSTP
GO TO 10
40 YAV=0.0
ISTART=ILOW
DO 45 J=ILOW,IHIGH
YAV=YAV+YH(J)
45 CONTINUE
CAPH(NUMB)=(HHIGH+HLOW)/2.0
CAPYH(NUMB)=(YAV-(YH(ILOW)+YH(IHIGH))/2.)/(IHIGH-ILOW)
HLOW = HLOW + WNDSTP
HHIGH = HLOW + WINDOW
IF (HHIGH LE H(NH)) GO TO 20
GO TO 70

FIND AVERAGE OF CONSECUTIVE PAIRS OF PEAKS
(A MINIMUM AND A MAXIMUM)

50 CALL MINMAX(H, YH, NH, HL, YHL, NL, HH, YHH, NK, 0)
NUMB = NL
IF ((NL - NK) GE 0.) NUMB = NK
DO 55 I = 1, NUMB
CAPYH(I) = (YHL(I) + YHH(I)) / 2.0
CAPH(I) = (HL(I) + HH(I)) / 2.0
55 CONTINUE
GO TO 70

TAKE ALL VALUES NO OSCILLATORY PART

60 NUMB = NH
DO 65 I = 1, NH
CAPYH(I) = YH(I)
CAPH(I) = H(I)
65 CONTINUE

WRITE (3, 402) (CAPH(I), CAPYH(I), I = 1, NUMB)
DO 75 IJK = 1, NUMB
CAPH(IJK) = CAPH(IJK) * CAPH(IJK)
IF (JUMP EQ 0) CAPYH(IJK) = CAPYH(IJK) / CAPH(IJK)
75 CONTINUE
CALL LSTSQU(CAPH, CAPYH, NUMB, MORDER, B, C, SUMD, SIGMA, KS)
IF (KS EQ 1) GO TO 9999
WRITE (3, 403) (B(J), J = 1, MP1)
DO 85 I = 1, NUMB
XC = CAPH(I)
CAPH(I) = SQRT(CAPH(I))
XCT = XC
YCAP = B(1)
DO 80 J = 2, MP1
YCAP = YCAP + B(J) * XC
XC = XC * XCT
80 CONTINUE
CAPYH(I) = YCAP
IF (JUMP EQ 0) CAPYH(I) = YCAP * XCT
85 CONTINUE
IF (NPLTDT EQ 1) GO TO 90
CALL YGRAPH(H, YH, NH, 'DATA', 4, 1, 1)
CALL SETI(4)
CALL YGRAPH(CAPH, CAPYH, NUMB, 'DATA', 4, 2, 99)
CALL SETI(-1)
90 CONTINUE
WRITE (3, 404) (CAPH(I), CAPYH(I), I = 1, NUMB)
SUBROUTINE SOLA

C PURPOSE: FIND SOLUTION FOR ALPHA AND AMPLITUDE

C USAGE: CALL SOLA

C METHOD

BASELINE IS SUBTRACTED FROM DATA, DATA CORRECTED
TO BE A PURE DAMPED SINUSOID. THE TRANSFORM IS
DONE, EXTREMUMS OF POWER SPECTRUM FOUND, AND A
SOLUTION FOR ALPHA AND THE AMPLITUDE TERM IS TRIED.
THEN ANOTHER METHOD FOR FINDING SAME PARAMETERS
IS DONE, THIS WINDOW ROUTINE FITS TO DATA PROPER.

COMMON/A/SINFT(1000),COSFT(1000)
COMMON/B/HI(2500),YHI(2500),NHI
COMMON/C/OMEG(450),RFT(450),UFT(450),PWR(450),NFT
COMMON/D/NPLTHI,NPLTPS,NTRANS
COMMON/E/NPLTDI,IBASE,MORDER,NOPLT,YO
COMMON/F/DOMEGA,OMEGAL,OMEGAU,IMPOSE
COMMON/G/B(10),C(10),SUMDF,SIGMA
COMMON/H/YSCALE,IDENT,ISWEEP,HFLOW,HFHIGH,MAG
COMMON/WK1/AMP(2500),PHA(2500),HIA(2500),ALOGA(2500)
COMMON/WK2/WLO(100),PLO(100),WHI(100),PHI(100)
DIMENSION A(400),RHS(20),FREQ(10)

C

TWOPI=6.283185

C

SUBTRACT BASELINE, MULTIPLY BY PROPER POWER OF
H TO GIVE DAMPED SINUSOID, AND INVERT H TO GET
1/H - HINVERSE

M1=MORDER+1
DO 60 I=1,NHI
HVI=HI(I)
H2=HVI*HVI
YSUB=0.0
DO 50 J=1,M1
YSUB=YSUB+B(J)*H2
H2=H2*HVI*HVI
50 CONTINUE
AMP(I)=(YHI(I)-YSUB)/SQRT(HVI)
IF(MAG.EQ.1) AMP(I)=AMP(I)*HVI*HVI*HVI
HIA(I)=1.0/HVI
60 CONTINUE
DO 70 I=1,NHI
K=NHI-I+1
HI(I)=HIA(K)
YHI(I)=AMP(K)
70 CONTINUE
REALL=HI(NHI)-HI(1)
C
NOW WE HAVE YH AS A FUNCTION OF 1/H IN THE FORM:
C
AMPLITUDE * EXP ( -ALPHA/H ) COS ( W/H + PHI)
C
NOW DO THE TRANSFORM OF YH(1/H), NHI DATA POINTS,
IMPOSE SAYS HOW MANY FREQUENCY COMPONENTS
TRANSFORM DONE BY CALCULATING WX = 2PI F AND
DIVIDING BY 2PI, HENCE WILL ONLY CALCULATE FX
C
IF(NPLTHI.EQ.1) GO TO 80
CALL SETX(17.0,1.0)
CALL YGRAPH(HI,YHI,NHI,'DATA - Y VS 1/H ',16,1,0)
80 W=OMEGAL/REAL
DFREQ=DOMEGA/REAL
FREQU=OMEGA/REAL
NFT=0
85 CALL TRANS(W,DFREQ,FREQU)
NFTSAV=NFT
IF(NPLTPS.EQ.1) GO TO 90
CALL SETX(12.0,1.0)
CALL SETY(11.0,0.5)
CALL YGRAPH(OMEG,PWR,NFT,'SPEC VS OMEG',12,1,0)
CALL SETX(17.0,1.0)
90 CONTINUE
WRITE(3,1009) (J,RFT(J),UFT(J),PWR(J),OMEG(J),J=1,NFT)
CALL MINMAX(OMEG,PWR,NFT,WLO,PLO,NLOW,WHI,PHI,NHIGH,1)
WRITE(3,800) (WLO(J),PLO(J),J=1,NLOW)
WRITE(3,800) (WHI(J),PHI(J),J=1,NHIGH)
WRITE(3,801) NHIGH,NLOW
800 FORMAT(/,(4El8.8))
801 FORMAT(2110)
C
C FIND THE MAX OF PHI AND ITS SUBSCRIPT
C
DO 110 JK=1,IMPOSE
  PWRMAX=PHI(JK)
  NCNTR=JK
  OMEGAC=WHI(JK)
  JKP1=JK+1
95 DO 100 J=JKP1,NHIGH
  IF(PHI(J).LT.PWRMAX) GO TO 100
  PWRMAX=PHI(J)
  OMEGAC=WHI(J)
  NCNTR=J
100 CONTINUE

C CALCULATE ALPHA & AMP FOR THIS FRQ COMP
C
OMEGAC=OMEGAC/TWOPI
CALL TRANS(OMEGAC,OMEGAC,OMEGAC)
PWRMAX=PWR(NFT)
RATIO=UFT(NFT)/RFT(NFT)
PHASE=ATAN(RATIO)
PERIOD=1000./OMEGAC
WEWCPP=OMEGAC+1.0/REALF
CALL TRANS(WEWCPP,WEWCPP,WEWCPP)
R1=PWR(NFT)/PWRMAX
WEWCMP=OMEGAC-1.0/REALF
CALL TRANS(WEWCMP,WEWCMP,WEWCMP)
R2=PWR(NFT)/PWRMAX
ALPHA=TWOPI*SQRT(SQRT(R1*R2/(1.0-R1)/(1.0-R2)))/REALF
HIAL=ALPHA*(HI(NHI)+HI(1))*0.5
AMPLIT=YSCALE*ALPHA*SQRT(PWRMAX)*EXP(HIAL)
AMPLIT=AMPLIT/SINH(ALPHA*REALF*0.5)
FREQ(JK)=OMEGAC
OMEGAC=OMEGAC*TWOPI
PWRMAX=PWRMAX*YSCALE*YSCALE
WRITE(3,1010) PWRMAX,OMEGAC,PERIOD,ALPHA,AMPLIT,
RATIO,PHASE
IF(NCNTR.EQ.JK) GO TO 110
PJK=PHI(JK)
WJK=WHI(JK)
PHI(JK)=PHI(NCNTR)
WHI(JK)=WHI(NCNTR)
PHI(NCNTR)=PJK
WHI(NCNTR)=WJK
110 CONTINUE

C ORDER FREQUENCIES - INCREASING
C
IF(IMPOSE.EQ.1) GO TO 123
DO 115 J=2,IMPOSE
  IT=IMPOSE+2-J
DO 115 I=2,IMPOSE
  IF(FREQ(I-1).LE.FREQ(I)) GO TO 115
  FREQMN=FREQ(I)
  FREQ(I)=FREQ(I-1)
  FREQ(I-1)=FREQMN
115 CONTINUE
CONTINUE
FREQMN=FREQ(2)-FREQ(1)
IF(IMPOSE.EQ.2) GO TO 122
DO 120 J=3,IMPOSE
IF(FREQ(J)-FREQ(J-1).GE.FREQMN) GO TO 120
FREQMN=FREQ(J)-FREQ(J-1)
120 CONTINUE
C WINDOW = 0.8 OF LONGEST DIFFERENCE PERIOD - OR -
C 20% OF DELTA(1/H)
C
122 HIWIN=0.8/FREQMN
IF(HIWIN.GT.0.2*REALL) HIWIN=0.2*REALL
GO TO 125
C WINDOW = 5 TIMES ONLY PERIOD
C
123 HIWIN=5.0/FREQ(1)
125 HIINC=HIWIN*0.4
HILow=HI(1)
HIHIGH=HILow+HIWIN
C FIND SUBSCRIPTS FOR WINDOW KWIN
C
M1=0
K1=IMPOSE
N2=IMPOSE*2
KWIN=0
130 M1=M1+1
IF(HI(M1).LT.HILOW) GO TO 130
M2=M1
135 M2=M2+1
IF(HI(M2).LE.HIHIGH) GO TO 135
M2=M2-1
C INITIALIZE MATRIX TO 0.0
C
DO 140 I=1,N2
RHS(I)=0.0
DO 140 J=1,N2
A((I-1)*N2+J)=0.0
140 CONTINUE
C CALCULATE ENTRIES OF MATRIX FOR THIS WINDOW
C
DO 150 K=M1,M2
DO 150 I=1,IMPOSE
ARG=FREQ(I)*HI(K)
NARG=ARG
AARG=NARG
JARGIK=(ARG-AARG)*1000.0+1
145 RHS(I)=RHS(I)+YHI(K)*COSFT(JARGIK)
RHS(I+IMPOSE)=RHS(I+IMPOSE)+YHI(K)*SINFT(JARGIK)
DO 150 J=1,N2,2
ARG=FREQ(J/2+1)*HI(K)
NARG=ARG
AARG=NARG
JARGJK=(ARG-AARG)*1000.0+1.0
KSUB=I+J*N2
A(KSUB-N2)=A(KSUB-N2)+COSFT(JARGJK)*COSFT(JARGIK)
A(KSUB)=A(KSUB)+SINFT(JARGJK)*COSFT(JARGIK)
A(KSUB-KI)=A(KSUB-KI)+COSFT(JARGJK)*SINFT(JARGIK)
A(KSUB+KI)=A(KSUB+KI)+SINFT(JARGJK)*SINFT(JARGIK)
CONTINUE
C
SOLVE AND FIND AMP AND PHASE FOR THIS WINDOW
C
CALL SIMQ(A,RHS,N2,KS)
IF(KS.EQ.0) GO TO 153
WRITE(3,1014)
GO TO 158
153 KWIN=KWIN+1
DO 155 I=1,IMPOSE
AMP(KWIN*KI-KI+I)=RHS(I)*RHS(I)+RHS(I+KI)*RHS(I+KI)
AMP(KWIN*KI-KI+I)=YSLE*SQRT(AMP(KWIN*KI-KI+I))
PHA(KWIN*KI-KI+I)=ATAN(-RHS(I+KI)/RHS(I))
CONTINUE
HIA(KWIN)=(HI(M1)+HI(M2))*0.5
C
MOVE WINDOW
C
158 HILOW=HILOW+HIINC
HIHIGH=HILOW+HIWIN
160 IF(HIHIGH.LE.HI(NHI)) GO TO 130
IF(KWIN.EQ.0) GO TO 190
DO 165 J=1,KWIN
M=(J-1)*KI
WRITE(3,1011) HIA(J),(AMP(M+I),PHA(M+I),I=1,KI)
CONTINUE
C
SOLVE FOR AMP AND ALPHA
C
DO 175 I=1,IMPOSE
DO 170 J=1,KWIN
ALOGA(J)=ALOG(AMP((J-1)*KI+I))
CONTINUE
CALL SETY(6.0,1.0)
CALL SETX(10.0,1.0)
CALL YGRAPH(HIA,ALOGA,KWIN,'FIT',4,1,0)
CALL LSTSQU(HIA,ALOGA,KWIN,1,B,C,SUMDIF,SIGMA,KS)
B(1)=EXP(B(1))
C(1)=YSLE*C(1)
WRITE(3,1015) FREQ(I),B(1),C(1),B(2),C(2),SIGMA,KS
CONTINUE
READ(1,1012) DOMEGA,OMEGAL,OMEGAU,IMPOSE
IF(DOMEGA.GT.0.0) GO TO 80
SUBROUTINE TRANS(F,DFREQ,FREQU)

C PURPOSE: DO FOURIER TRANSFORM: F TO FREQU

C USAGE: CALL TRANS(F,DFREQ,FREQU)

C DESCRIPTION OF PARAMETERS

C
C F - FIRST VALUE OF FREQUENCY
C
C DFREQ - STEP FREQUENCY
C
C FREQU - LAST VALUE OF FREQUENCY FOR TRANSFORM
C
C METHOD

C

C FOURIER TRANSFORM IS CALCULATED BY TRAPEZOIDAL
C INTEGRATION, AND USING TRIG TABLES STORED IN COMMON
C
COMMON/A/SINFT(1000),COSFT(1000)
COMMON/B/HI(2500),YHI(2500),NHI
COMMON/C/OMEGA(450),RFT(450),UFT(450),PWRSPT(450),NFT

C

C CALCULATE CONTRIBUTION FROM END POINTS

C

W=F
AMP1=(HI(2)-HI(1))*YHI(1)*0.5
AMP2=(HI(NHI)-HI(NHI-1))*YHI(NHI)*0.5
10 ARG=W*HI(1)
   NARG=ARG
   AARG=NARG
   JARG1=(ARG-AARG)*1000.0+1.0
   ARG=W*HI(NHI)
   NARG=ARG
   AARG=NARG
   JARG2=(ARG-AARG)*1000.0+1.0
   ASUM=AMP1*COSFT(JARG1)+AMP2*COSFT(JARG2)
   BSUM=AMP1*SINFT(JARG1)+AMP2*SINFT(JARG2)
   NHIM1=NHI-1

   NOW DO TRANSFORM OVER REST OF DATA RANGE

   DO 20 I=2,NHIM1
      ARG=W*HI(I)
      NARG=ARG
      AARG=NARG
      JARG=(ARG-AARG)*1000.0+1.0
      AMP=(HI(I+1)-HI(I-1))*YHI(I)*0.5
      ASUM=ASUM+AMP*COSFT(JARG)
      BSUM=BSUM+AMP*SINFT(JARG)
   20 CONTINUE
   NFT=NFT+1
   RFT(NFT)=ASUM
   UFT(NFT)=BSUM
   PWRSPN(NFT)=ASUM*ASUM+BSUM*BSUM
   OMEGA(NFT)=W*6.283185
   W=W+DFREQ
   IF(W.LE.FREQU) GO TO 10
RETURN
END

SUBROUTINE MINMAX(X,Y,N,XL,YL,NL,XH,YH,NH,IFIT)

PURPOSE: FIND EXTREMUMS OF VECTOR (X,Y)

USAGE: CALL MINMAX( LIST )

DESCRIPTION OF PARAMETERS

X,Y,N - VECTOR OF DATA
XL,YL,NL - VECTOR OF MINIMUMS
XH,YH,NH - VECTOR OF MAXIMUMS
IFIT =1FIT EXTREMUM TO QUADRATIC = SPACED DATA
     =OTAKE EXTREMUM POINTS IN DATA

DIMENSION X(N),Y(N),XL(N),YL(N),XH(N),YH(N)
NL=0
NH=0
NN=N-1
DO 10, I=1,NN
    IF(Y(I+1).NE.Y(I)) GO TO 15
10 CONTINUE
    GO TO 100
15 K=I
    IF(Y(I+1).GT.Y(I)) GO TO 40
    DO 20 K=I,NN
    IF(Y(K+1).GT.Y(K)) GO TO 25
20 CONTINUE
    GO TO 100
25 NL=NL+1
    XL(NL)=X(K)
    YL(NL)=Y(K)
    IF(IFIT.EQ.0) GO TO 40
30 A3=Y(K-1)-2.0*Y(K)+Y(K+1)
    DX=(X(K+1)-X(K-1))/2.0
    A2=-2.0*A3*X(K)+DX*(Y(K+1)-Y(K-1))
    A1=X(K)*X(K)*A3+X(K)*B*Y(K-1)+2.0*Y(K)*DX*DX
    XL(NL)=-0.5*A2/A3.
    YL(NL)=(A1-0.25*(A2/A3)*A2)/2.0/DX/DX
    GO TO 40
40 DO 50 I=K,NN
    IF(Y(I+1).LT.Y(I)) GO TO 60
50 CONTINUE
    GO TO 100
60 NH=NH+l
    XH(NH)=X(I)
    YH(NH)=Y(I)
    IF(IFIT.EQ.0) GO TO 15
70 A3=Y(I-L)-2.0*Y(I)+Y(I+1)
    DX=(X(I+1)-X(I-1))/2.0
    A2=-2.0*A3*X(I)+DX*(Y(I+1)-Y(I-1))
    A1=X(I)*X(I)*A3+X(I)*B*Y(I-1)+2.0*Y(I)*DX*DX
    XH(NH)=-0.5*A2/A3.
    YH(NH)=(A1-0.25*(A2/A3)*A2)/2.0/DX/DX
    GO TO 15
100 RETURN
END

SUBROUTINE LSTSQU(X,Y,N,M,B,C,SUMD,RMSD,KS)

PURPOSE

TO FIND COEFFICIENTS OF POLYNOMIAL FIT TO DATA
BY LEAST SQUARES

USAGE: CALL LSTSQU( LIST )

DESCRIPTION OF PARAMETERS

X,Y,N - VECTOR OF N DATA POINTS TO BE FIT
M - ORDER OF POLYNOMIAL
RESULTING COEFFICIENTS FOR POLYNOMIAL

VARIATION OF COEFFICIENTS

SUM OF DIFFERENCES AT EACH POINT

ROOT MEAN SQUARE DEVIATION

CONDITION CODE FROM SIMQ, 0-PROPER SOLUTION

1-SINGULAR SOLUTION

DIMENSION X(N), Y(N), A(10,10), W(150), B(1), C(1)

IF(M.GE.N) M=N-1

YEXP10=10.0**(IFIX(ALOG10(ABS(Y(N)))))

XEXP10=X(N)

DO 10 I=1,N

Y(I)=Y(I)/YEXP10

X(I)=X(I)/XEXP10

10 CONTINUE

M1=M+1

M2=2*M+1

DO 15 I=1,M2

W(I)=0.0

IF(I.LE.M1) B(I)=0.0

15 CONTINUE

CALCULATE AUGMENTED MATRIX

DO 20 K=1,N

P=1.0

DO 20 I=1,M2

W(I)=W(I)+P

IF(I.LE.M1) B(I)=B(I)+Y(K)*P

P=P*X(K)

20 CONTINUE

DO 25 I=1,M1

DO 25 J=1,M1

A(I,J)=Q(I+J-1)

25 CONTINUE

WRITE(3,100) ((A(I,J),J=1,M1),I=1,M1)

WRITE(3,100) (B(J),J=1,M1)

100 FORMAT(//,(6E18.8))

CALL DETER(A,M1,DETSAV)

IF(DETSAV.EQ.0.0) DETSAV=1.0E+50

DETF=DETSAV

CALCULATE DETERMINANT OF COFACTOR MATRICES

DO 35 K=1,M1

L=0

DO 30 I=1,M1

IF(I.EQ.K) GO TO 30

LM=0

L=L+1

DO 30 J=1,M1

IF(J.EQ.K) GO TO 30

LM=LM+1

A(L,LM)=W(I+J-1)

30 CONTINUE
CALL DETER(A,L,DETSAV)
C(K)=DETSAV
35 CONTINUE
WRITE(3,100) (C(K),K=1,M1),DET
C
C
SET UP AND SOLVE FOR COEFFICIENTS
C
MSQU=M1*M1
DO 40 I=1,M2
W(MSQU+I)=W(I)
40 CONTINUE
DO 45 J=1,M
MXM=J*M1
MM=MSQU+J
DO 45 I=1,M1
W(MXM+I)=W(MM+I)
45 CONTINUE
CALL SIMQ(W,B,M1,KS)
IF(KS.EQ.1) GO TO 9999
C
C
RESHUFFLE DATA AND COEFFICIENTS
C
DO 50 I=1,M1
B(I)=B(I)*YEXP10/(XEXP10**(I-1))
C(I)=C(I)/(XEXP10**(2*(I-1)))
50 CONTINUE
RMSD=0.0
SUMD=0.0
DO 60 I=1,N
Y(I)=Y(I)*YEXP10
X(I)=X(I)*XEXP10
DIF=Y(I)-B(I)
DO 55 J=2,M1
DIF=DIF-B(J)*X(I)**(J-1)
55 CONTINUE
SUMD=SUMD+DIF
RMSD*RMSD+DIF*DIF
60 CONTINUE
RMSD=SQRT(RMSD/N)
DO 65 I=1,M1
C(I)=RMSD*SQRT(ABS(C(I)*N/DET/(N-M1)))
65 CONTINUE
9999 RETURN
END

SUBROUTINE DETER(A,N,DET)
C
PURPOSE: CALCULATE DETERMINANT OF A
C
USAGE: CALL DETER(A,N,DET)
DESCRIPTION OF PARAMETERS

A - SQUARE MATRIX
N - SIZE OF A
DET - RESULTANT DETERMINANT

METHOD: PIVOTAL ON LARGEST ELEMENT IN A COLUMN

DIMENSION A(10,10)
IF(N.GT.1) GO TO 15
DET=A(1,1)
RETURN
15 NMIN1=N-1
XCHANG=1.0
DET=1.0
DO 50 I=1,NMIN1
IPLUS1=I+1

FIND LARGEST ELEMENT IN COLUMN I

ATEST=A(I,I)
LROW=I
DO 20 J1=IPLUS1,N
IF(ATEST.GE.A(J1,I)) GO TO 20
ATEST=A(J1,I)
LROW=J1
20 CONTINUE
IF(ABS(ATEST).GE.1.0E-20) GO TO 21
DET=0.0
RETURN
21 IF(LROW.EQ.I) GO TO 35
XCHANG=XCHANG*(-1.0)

INTERCHANGE ROWS I AND LROW

22 DO 30 J2=1,N
ATEMP=A(I,J2)
A(I,J2)=A(LROW,J2)
A(LROW,J2)=ATEMP
30 CONTINUE
35 AII=A(I,I)
DET=DET*AI1
DO 40 K=IPLUS1,N
QUOTE=A(K,I)/AI1
DO 40 J=I,N
A(K,J)=A(K,J)-QUOTE*A(I,J)
40 CONTINUE
50 CONTINUE
DET=DET*A(N,N)*XCHANG
RETURN
END
SUBROUTINE YGRAPH(X,Y,N,LABEL,NLABEL,IC,IRPT)

C PURPOSE: PLOT THE VECTOR X-Y
C
USAGE: CALL YGRAPH( LIST )
C
DESCRIPTION OF PARAMETERS
C
X,Y,N - VECTOR OF N POINTS TO BE PLOTTED
LABEL - IDENTIFYING NAME OF NLABEL CHARACTERS
IC - PEN CONTROL, 1-PEN UP, 2-PEN DOWN BETWEEN PTS.
IRPT - =0 ONLY ONE PLOT ON PAGE
>0 MULTIPLE PLOTS PER PAGE:  1=FIRST PLOT,
2-98=INTERMEDIATE PLOTS, 99=LAST PLOT.
C
NOTES: PENPOSE MUST BE CALLED BEFORE FIRST CALL AND
LSTPLT MUST BE CALLED AFTER LAST CALL TO
YGRAPH. SUBROUTINE SET IS USED TO INITIALIZE
PLOT PAGE PARAMETERS
C
COMMON/GRAPH/YLONG,YMARG,XLONG,XMARG,XDEL,YDEL,ISYM
DIMENSION X(N),Y(N),LABEL(1)
IF(IRPT.GT.1) GO TO 30
IF(XLONG.GT.17.0.OR.XLONG.LE.2.0) XLONG=17.0
IF(YLONG.GT.11.0.OR.YLONG.LE.3.0) YLONG=11.0
IF(YMARG.GE.YLONG*.5-.5.OR.YMARG.LE.0.) YMARG=1.0
IF(XMARG.GE.XLONG*.5.OR.XMARG.LE.0.) XMARG=1.0
CALL EXTRMA(X,N,XMARG,XLONG,XMIN,XMAX,XORG,XDEL,IRPT)
CALL EXTRMA(Y,N,YMARG,YLONG,YMIN,YMAX,YORG,YDEL,-1)
CALL NEWPLT(XMARG,YORG,XLONG)
CALL ORIGIN(XMIN,0.0)
CALL XSCALE(XMIN,XMAX,XLONG-2*XMARG)
CALL YSCALE(YMIN,YMAX,YLONG-2*YMARG)
CALL XAXIS(10.0**XDEL)
CALL YAXIS(10.0**YDEL)
IF(ISYM.LT.-1.OR.ISYM.GT.14) ISYM=-1
IF(ISYM.EQ.-1.AND.IC.EQ.2) ISYM=11
J=N
GO TO 45
30 J=0
DO 40 I=1,N
IF(Y(I).GT.YMAX.OR.Y(I).LT.YMIN) GO TO 40
IF(X(I).GT.XMAX.OR.X(I).LT.XMIN) GO TO 40
J=J+1
Y(J)=Y(I)
X(J)=X(I)
40 CONTINUE
45 CALL XYPLT(X,Y,J,IC,ISYM)
IF(IRPT.GE.1.AND.IRPT.NE.99) GO TO 50
NLR=NLABEL/4
WRITE(3,100) XDEL,XMIN,XMAX,YDEL,YMIN,YMAX,(LABEL(J),
1J=1,NLR)
100 FORMAT(/,20X,'XSCALE=1.E',F4.0,2F20.10,/,20X,
SUBROUTINE SET

PURPOSE

TO ALLOW PROGRAM TO CHANGE PLOT PAGE PARAMETERS

USAGE

CALL SETY(YLONG,YMARG)
CALL SETX(XLONG,XMARG)
CALL SETI(ISYM)

DESCRIPTION OF PARAMETERS

YLONG - LENGTH OF Y AXIS IN INCHES
YMARG - Y MARGIN IN INCHES
XLONG - LENGTH OF X AXIS IN INCHES
XMARG - X MARGIN IN INCHES
ISYM - CODE FOR SYMBOL TO BE PLACED AT EACH POINT

COMMON/GRAPH/A1,A2,A3,A4,A8,A9,K10
ENTRY SETY(YLONG,YMARG)
A1=YLONG
A2=YMARG
RETURN
ENTRY SETX(XLONG,XMARG)
A3=XLONG
A4=XMARG
RETURN
ENTRY SETI(ISYM).
K10=ISYM
RETURN
END

SUBROUTINE EXTRMA(B,N,BMRG,BLNG,BMIN,BMAX,BORG,BDEL,J)

PURPOSE

TO FIND EXTREMA OF B AND SET PLOT PARAMETERS

USAGE: CALL EXTRMA( LIST )
DESCRIPTION OF PARAMETERS

B - NAME OF CURRENT AXIS
N - NUMBER OF POINTS
BMRG - MARGIN OF B AXIS
BLNG - LENGTH OF B DIMENSION ON PLOT PAGE
BMIN - MINIMUM VALUE OF B TO BE PLOTTED
BMAX - MAXIMUM VALUE OF B TO BE PLOTTED
BORG - VALUE OF ORIGIN OF B AXIS
BDEL - INCREMENT OF TICK MARKS FOR AXIS
J - CONTROL PARAMETER

DIMENSION B(N)
GRINT(A)=AINT(A)*SIGN(.5,A)-.5
BMAX=B(1)
BMIN=B(1)
DO 1 I=2,N
BMAX=AMAX1(BMAX,B(I))
BMIN=AMIN1(BMIN,B(I))
1 CONTINUE
AMIN=10.0***(GRINT(ALOG10(ABS(BMIN))))
IF(AMIN.LT.1.0) AMIN=0.1*AMIN
K=0
30 K=K+1
IF(K*AMIN.LE.ABS(BMIN)) GO TO 30
BMIN=(K-1)*AMIN*SIGN(1.0,BMIN)
IF(BMIN.LT.0.0) BMIN=BMN-AMIN
AMAX=10.0***(GRINT(ALOG10(ABS(BMAX))))
K=0
32 K=K+1
IF(K*AMAX.LT.ABS(BMAX)) GO TO 32
BMAX=K*AMAX*SIGN(1.0,BMAX)
IF(J.GE.1.AND.BMIN.GT.0.0) BMIN=0.0
IF(J.EQ.-1.AND.BMIN.GT.0.0) BMIN=0.0
25 IF(BMAX.LT.0.0) BMAX=0.0
BRANGE=BMAX-BMIN
BORG=BMN-BMIN*(BLNG-2*BMRG)/BRANGE
BRANGE=BRANGE/10.
BDEL=GRINT(ALOG10(ABS(BRANGE)))
RETURN
END
VII. BIBLIOGRAPHY

1. J. P. Joule, Phil. Mag. Ser. 3 30, 76 and 225 (1847).
17. A. D. C. Grassie, Phil. Mag. 9, 847 (1964).

19. An expanded discussion of the experimental details may be found in Appendices A and B of Ph. D. dissertation of J. M. Carter, University of Missouri - Rolla, (1970).


22. D. M. Sparlin, to be published.


35. The sample with $\varepsilon_{[0001]}$ and the sample with $\varepsilon_{[10\overline{1}0]}$ were cut from different boules which may account for the different value of "kink" field with $H$ parallel to $[0001]$.


VIII. VITA

James Milo Carter was born in Aurora, Missouri on December 16, 1944. He received his elementary education from Lowell Grade School and his secondary education from Aurora Jr-Sr High School, graduating in 1962. He then enrolled in the University of Missouri at Rolla in 1962 and earned a Bachelor of Science in Electrical Engineering in 1966. He was granted a Master of Science in Physics in 1968, again from the University of Missouri - Rolla.

He is married to the former Sharon Steele of Bethesda, Maryland. They have one son, Henry James.