SHIFT MEASUREMENTS OF THE STARK-BROADENED
IONIZED HELIUM LINES AT 1640 AND 1215 Å

by

James R. Van Zandt

Thesis submitted to the Faculty of the Graduate School of the University of Maryland in partial fulfillment of the requirements for the degree of Doctor of Philosophy 1976
ABSTRACT

Title of Dissertation: SHIFT MEASUREMENTS OF THE STARK-BROADENED IONIZED HELIUM LINES AT 1640 AND 1215 Å

James Russell Van Zandt, Doctor of Philosophy, 1976

Dissertation directed by: Hans R. Griem, Professor of Physics

Time-resolved measurements were made of the shifts of the ionized helium lines at 1640 Å (n = 3 → 2) and 1215 Å (n = 4 → 2), and of the Stark profile of the λ 1215 Å line. An electromagnetic shock tube was used as a light source. The plasma conditions corresponded to electron temperatures of ≈3.5 eV and electron densities of 0.8 to 1.8 × 10^{17} cm^{-3}. The measured shifts fell between two previous estimates of plasma polarization shifts. The measured Stark width of the λ 1215 Å line was up to 30% greater than the theoretical width.
DEDICATION

To my wife, Nita, who kept my nose to the grindstone.
ACKNOWLEDGMENTS

I would like to express my gratitude to Prof. H. R. Griem for suggesting the topic of this dissertation and for guidance throughout, to Drs. Larry Jones, Walter W. Jones, and Manfred Neiger for many helpful discussions, to Mr. Elmer Pierpont for his expert advice and assistance in the fabrication of equipment, to Mrs. Clara Rodriguez for her cheerful help in ordering materials and supplies, and to Mrs. Janet Wolfsheimer for typing the manuscript. Without their help, it would not have been possible to finish this work.

This work was supported by funds from the National Aeronautics and Space Administration and the National Science Foundation.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEDICATION</td>
<td>ii</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. THEORETICAL BACKGROUND.</td>
<td>3</td>
</tr>
<tr>
<td>A. Line Intensities</td>
<td>3</td>
</tr>
<tr>
<td>B. Continuum Intensities</td>
<td>7</td>
</tr>
<tr>
<td>C. Radiation Transfer</td>
<td>10</td>
</tr>
<tr>
<td>D. Line Broadening</td>
<td>11</td>
</tr>
<tr>
<td>E. Validity of LTE</td>
<td>18</td>
</tr>
<tr>
<td>III. EXPERIMENTAL METHOD</td>
<td>21</td>
</tr>
<tr>
<td>A. Apparatus</td>
<td>21</td>
</tr>
<tr>
<td>1. T-tube and circuit</td>
<td>21</td>
</tr>
<tr>
<td>2. VUV monochromator and detector</td>
<td>25</td>
</tr>
<tr>
<td>3. Visible monochromators and detectors</td>
<td>25</td>
</tr>
<tr>
<td>B. Data Reduction</td>
<td>27</td>
</tr>
<tr>
<td>IV. RESULTS AND DISCUSSION</td>
<td>29</td>
</tr>
<tr>
<td>A. Results</td>
<td>29</td>
</tr>
<tr>
<td>B. Discussion of Possible Errors</td>
<td>35</td>
</tr>
<tr>
<td>1. Impurity lines</td>
<td>35</td>
</tr>
<tr>
<td>2. Wavelength standards</td>
<td>38</td>
</tr>
<tr>
<td>3. He II 1215 asymmetry</td>
<td>38</td>
</tr>
<tr>
<td>4. Departure from LTE</td>
<td>39</td>
</tr>
<tr>
<td>5. Summary of errors</td>
<td>40</td>
</tr>
</tbody>
</table>
C. Discussion of Results. ........................................ 41
D. Conclusions and Suggestions. ............................. 43

APPENDIX A. WAVEFORM RECORDER ......................... 45
APPENDIX B. STATISTICS. ...................................... 51
APPENDIX C. PROGRAMS. ....................................... 53
REFERENCES .................................................. 126
LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-1</td>
<td>Plasma Conditions, Shifts of He II $\lambda$ 1640 Å</td>
<td>34</td>
</tr>
<tr>
<td>4-2</td>
<td>Plasma Conditions, Shifts and Widths of He II $\lambda$ 1215 Å</td>
<td>37</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-1</td>
<td>Calculated helium ionization stage concentrations</td>
<td>4</td>
</tr>
<tr>
<td>2-2</td>
<td>Calculated conditions for a pure helium plasma</td>
<td>5</td>
</tr>
<tr>
<td>2-3</td>
<td>Calculated helium line intensities</td>
<td>8</td>
</tr>
<tr>
<td>2-4</td>
<td>Holtsmark field strength distribution</td>
<td>16</td>
</tr>
<tr>
<td>2-5</td>
<td>Holtsmark profile for the H_b line (broadened only by statistically uncorrelated ions)</td>
<td>17</td>
</tr>
<tr>
<td>3-1</td>
<td>T-tube schematic</td>
<td>22</td>
</tr>
<tr>
<td>3-2</td>
<td>Experiment circuit diagram</td>
<td>22</td>
</tr>
<tr>
<td>3-3</td>
<td>Schematic of vacuum system</td>
<td>24</td>
</tr>
<tr>
<td>3-4</td>
<td>Schematic of optical arrangement</td>
<td>26</td>
</tr>
<tr>
<td>4-1</td>
<td>Measured and best-fit profile for He II λ 4686 Å line</td>
<td>30</td>
</tr>
<tr>
<td>4-2</td>
<td>Measured and best-fit profile for He II λ 1640 Å line</td>
<td>31</td>
</tr>
<tr>
<td>4-3</td>
<td>Measured and best-fit profile for He II λ 1215 line</td>
<td>32</td>
</tr>
<tr>
<td>4-4</td>
<td>Estimated and measured shifts of He II λ 1640 Å line</td>
<td>33</td>
</tr>
<tr>
<td>4-5</td>
<td>Estimated and measured shifts of He II λ 1215 Å line</td>
<td>36</td>
</tr>
<tr>
<td>4-6</td>
<td>Densitometer scan of spectrum near He II λ 4686 Å line</td>
<td>37a</td>
</tr>
<tr>
<td>4-7</td>
<td>Densitometer scan of spectrum near He II λ 1640 Å line</td>
<td>37b</td>
</tr>
<tr>
<td>4-8</td>
<td>Densitometer scan of spectrum near He II λ 1215 Å line</td>
<td>37c</td>
</tr>
<tr>
<td>A-1</td>
<td>Block diagram of waveform recorder</td>
<td>46</td>
</tr>
<tr>
<td>C-1</td>
<td>Record format of waveform recorder tape</td>
<td>56</td>
</tr>
<tr>
<td>C-2</td>
<td>Format of data record written by REVERT.</td>
<td>56</td>
</tr>
<tr>
<td>C-3</td>
<td>Format of data record written by PARAM or BSORT.</td>
<td>57</td>
</tr>
<tr>
<td>C-4</td>
<td>Format of plot-file data record written by PROFILE</td>
<td>57</td>
</tr>
<tr>
<td>C-5</td>
<td>Format of fit-file data record written by PROFILE</td>
<td>57</td>
</tr>
</tbody>
</table>

vii
Spectroscopy has long been recognized as an important diagnostic tool for both astrophysical plasmas, where it is often the only method available, and in the laboratory where, unlike many methods, it does not disturb the plasma under study.

The considerable theoretical and experimental efforts in this field have resulted in good understanding of the pressure broadening and shifts of spectral lines due to the Stark effect of nearby charged perturbers. Particular attention has been paid to the lines of hydrogen and the hydrogenic ions, for which the quasistatic and impact theories predict considerable broadening but no shifts. However, in 1962, Berg et al reported a blue shift for the He II 4686 line, which they attributed to the reduction of the Coulomb potential of the nucleus by the polarization of the plasma near the radiating ion. Later measurements demonstrated this "shift" had been simulated by some unresolved Si III lines on the blue wing of the helium line. Greig et al then reported blue shifts of the He II 304 line. Subsequent photographic measurements did not verify the shift of the 304 line, but higher series members (256, 243, etc.) had blue shifts which could have been due to plasma polarization. The most recent measurement showed blue shifts for the 256 and 243 lines, with a greater shift for the 304 line, in agreement with Greig's result.

The polarization shift is expected to be important for high-Z ion lines and may limit wavelength accuracies in, for example, laser-produced plasmas. The theoretical treatments of this effect have
been unsatisfactory,\textsuperscript{7,8} and no attempts have been made to measure shifts of the "Balmer" (or "second Lyman") series lines of ionized helium, at 1640, 1215, 1084 ... Å. The primary aim of this experiment was to look for such shifts, and investigate their possible dependence on plasma conditions. A secondary purpose was to measure the Stark broadening of the higher series members, to check the theoretical calculations.\textsuperscript{9,10}

A T-tube was chosen as a source because it produces a fairly homogeneous plasma\textsuperscript{6} near local thermal equilibrium (LTE),\textsuperscript{11,12} at a density and temperature suitable for the emission of ionized helium lines. The line positions were measured relative to nearby impurity lines. Plasma conditions were determined from photoelectric measurements of the He II 4686 line, and plasma reproducibility was checked by monitoring the total intensities of the 4686 line and the continuum near 4976 Å.

The first chapter of this dissertation has served as an introduction. In Chapter 2 some of the relevant results of plasma spectroscopy are presented. A description of the experimental apparatus and method appears in Chapter 3. The experimental results, with a discussion of them and possible errors, are in Chapter 4.
CHAPTER II

THEORETICAL BACKGROUND

A. Line Intensities

The relative intensities of emission lines depend on the population densities of atoms in the upper state and the probability of radiative transition to the corresponding lower state.

In equilibrium, the density \( N_z \) of ions of charge \( Z \) is related to the electron density \( N_e \) and the density of atoms in the next lower ionization stage according to the Saha equation\(^\text{13}\)

\[
\frac{N_e N_z}{N_{z-1}} = 2 \frac{Z_z(T)}{Z_{z-1}(T)} \left( \frac{m_e kT}{2\pi\hbar^2} \right)^{3/2} \exp \left( -\frac{E_{\infty}^{z-1} - \Delta E^{z-1}}{kT} \right) . \tag{2-1}
\]

Since nearly all the atoms are in the ground state, the partition function \( Z_z(T) \) can usually be replaced by the statistical weight \( g_z \) of the ground state. In this case, \( Z = 0 \), and we have

\[ g_z = \begin{cases} 2S+1 & \text{for } H^+, \text{He}^0, \text{He}^{++}; \\ 2 & \text{for } H^0 \text{ and He}^+ \end{cases} \]

The correction \( \Delta E_{\infty}^{z-1} \) to the ionization energy \( E_{\infty}^{z-1} \) due to Coulomb interactions in the plasma is\(^\text{13}\)

\[
\Delta E_{\infty}^{z-1} = \frac{Ze^2}{4\pi\epsilon_0 \lambda_D} , \tag{2-2}
\]

where \( \lambda_D \) is the plasma Debye length\(^\text{14}\)

\[
\lambda_D = \left( 4\pi \sum_{1} \frac{N_1 q_1^2}{kT_1} \right)^{-1/2} , \tag{2-3}
\]

where \( N_1 \) is the density of particles with charge \( q_1 \). Plots of helium ionization stage concentrations as functions of temperature appear in Fig. 2-1. Plots of \( \lambda_D \) and other plasma properties appear in Fig. 2-2.
Fig. 2-1 Calculated helium ionization stage concentrations
Fig. 2-2 Calculated conditions for a pure helium plasma
where the shaded region is typical of T-tubes. Note that the plasma approximation $N_e \lambda_D^3 \gg 1$ (indicating many particles in a Debye sphere) is only marginally satisfied.

The population densities $N_{nLS}$ of the state $(n,L,S)$ of a given ionization stage is given by the corresponding Boltzmann factor

$$N_{nLS} = g_{nLS} \exp \left(- \frac{E_{nLS}}{kT} \right), \quad (2-4)$$

together with the normalization condition. The exponential term is nearly always much less than one for excited states, justifying the earlier statement that most atoms are in the ground state. Note that an isolated atom has an infinite number of bound states, whose energies tend to the ionization energy $E_i$. When the atom is embedded in a plasma, however, the ionization energy is reduced as described above, and only a finite number of bound states remain.

Treating an atom as an electric dipole radiator, the transition probability per unit time for spontaneous emission is

$$A_{lu} = \frac{4e^2\omega^3}{3\hbar^2c^3[4\pi\varepsilon_0]} g_u \sum_i |\langle \xi_i | u \rangle|^2 \delta_{av}, \quad (2-5)$$

which is tabulated for many spectral lines. The sum is over the components of the coordinate vector of the radiating electron, and the average is over possible final states. Multiplying by the energy $\hbar\omega$ of the photon, and using (2-4) to relate the upper state population density to the ground state population density $N_g$ (with statistical weight $g_g$) we find the total power per unit volume spontaneously radiated in the given line to be

$$P_{lu} = 2\pi\hbar c \frac{N_g A_{lu} g_u}{\lambda g_g} \exp \left(- \frac{E_u}{kT} \right), \quad (2-6)$$
Since the line intensities are proportional to the concentration of atoms in the appropriate ionization stage, the intensity ratio of lines of different ionization states is an extremely sensitive function of temperature (see Fig. 2-3), and can be used to measure the temperature. Note, however, that this measurement depends strongly on the assumption of local thermal equilibrium, which can require a long time and considerable distance to establish between states with very different energies.

B. Continuum Intensities

Plasmas emit continuum radiation due to radiative recombination (inverse photoionization), bremsstrahlung, and the formation of negative ions. A pseudo-continuum results when the Stark profiles of nearby lines overlap.

The extremely weak bremsstrahlung radiation due to ion-ion and nonrelativistic electron-electron collisions can be neglected. That due to electron collisions with ions of charge $z$ is given by

$$
e = \frac{16\pi e^6}{3c^2 \sqrt{8\pi m_e}} \frac{N_e N_z}{z^2} G_z(\omega, T_e),$$

where $G_z$ is the free-free Gaunt factor, which is usually of order one.

The radiation from electron-neutral collisions (approximated by elastic, billiard-ball type interactions) is given by

$$
e = \frac{32e^2}{3c^3 (2\pi m_e)^{3/2}} \frac{N_e N_0 (kT_e)^{3/2}}{G_0(\omega, T)}.$$

When an ion captures a free electron, the binding energy and the electron's kinetic energy are given to a photon. For recombination into a given orbital $(n, L, S)$, the photon then has the minimum energy
Fig. 2-3 Calculated helium line intensities
\[ \tau = E_{z-1,n} - E_{z-1,n} . \] (2-9)

Viewed another way, this restricts the possible final states for the electron for a contribution to the continuum at a given frequency. The recombination continuum is then, by detailed balancing,\(^{16}\)

\[ \epsilon_R = \frac{2\pi \hbar^4}{c^2} \frac{N e^2 N}{(2\pi m e T_e)^{3/2}} \exp \left( \frac{-\hbar \omega}{kT_e} \right) \sum \frac{g_{z-1,n}}{g_{z,1}} \sigma_{z-1,n} , \] (2-10)

where \( \sigma_{z-1,n} \) is the photoionization cross section\(^{18,19}\), \( g_{z-1,n} \) and \( g_{z,1} \) are statistical weights, and the sum runs from the lowest allowed state to the highest bound state (i.e., with energy less than the reduced ionization energy calculated from (2-2)).

Some electronegative atoms (H, N, O, C, etc.) can capture a free electron and form a negative ion, while emitting a continuum as in recombination. The spectral emission coefficient is, similarly,\(^{16}\)

\[ \epsilon^- = \frac{2\pi \hbar^4}{c^2} \frac{N e^2 N}{(2\pi m e T_e)^{3/2}} \frac{\sigma^-}{Z_0(T_e)} \exp \left( \frac{-E_a - \hbar \omega}{kT_e} \right) , \] (2-11)

where \( \sigma^- \) is the statistical weight of the negative ion (which usually has only one bound state), \( Z_0 \) is the partition function of the neutral atom, \( E_a \) is the binding energy of the new electron (generally less than 2 eV), and \( \sigma^- \) is the cross section for the inverse process of photodetachment.\(^{20}\)

This process is unimportant in hot plasmas, where the density \( N_a \) of neutral atoms is low.

The pseudo-continuum of lines is generally important only for hydrogenic atoms, which are subject to the linear Stark effect, and then only near a series limit. The last clearly distinguishable line of a series is then given by the Inglis-Teller limit.\(^{21}\)

Since both line and continuum intensities increase with electron
density, but scale differently with temperature, the ratio of the line intensity to that of the nearby continuum can be used to measure the temperature.

C. Radiation Transfer

In previous sections we have discussed the spectral emission coefficient $\varepsilon_\omega$ of the plasma, expressed as power radiated per unit solid angle, frequency interval, and volume. The experimentally measurable quantity is $I_\omega$, the power radiated per unit solid angle, frequency interval, and surface area of plasma observed. In the simplest situation, i.e., neglecting scattering, it obeys the differential equation

$$\frac{d}{dx} I_\omega = \varepsilon_\omega - k'I_\omega,$$

where $k'_\omega$ is the effective absorption constant, equal to the actual absorption constant minus the induced emission. $\varepsilon_\omega$ includes only the spontaneous emission. If the plasma is in LTE, the emission follows Kirchoff's law

$$\varepsilon_\omega = k'B_\omega(T),$$

where $B_\omega$ is the Planck function. If we further assume the plasma to be homogeneous, the solution of (2-12) is

$$I_\omega(\xi) = B_\omega(T)[1 - \exp(-k'_\omega)] -$$

The quantity $k'_\omega\xi$ is the "optical depth", and if $k'_\omega \ll 1$, the equation reduces to

$$I_\omega(\xi) = B_\omega(T)k'_\omega = \varepsilon_\omega \xi,$$
as expected. In the opposite limit, \( k_\omega \gg 1 \), the plasma radiates as a blackbody. Stellar atmospheres have great optical depth at almost all wavelengths, while laboratory plasmas are normally optically thin except possibly near the centers of some resonance lines.

D. Line Broadening

Spectral line broadening in a plasma is a complex phenomenon, and no attempt is made here to discuss all the results of investigations in atomic spectroscopy, astrophysics, and plasma spectroscopy. Only a physical picture of the various effects is presented.

Let the (frequency-space) spectral line profile \( I(\omega) \) be proportional to the light intensity between \( \omega \) and \( \omega + d\omega \), subject to the normalization condition

\[
\int_{-\infty}^{\infty} I(\omega) d\omega = 1.
\]  
(2-16)

These spectral intensities are the squares of the corresponding Fourier components \( C(\omega) \):

\[
I(\omega) = |C(\omega)|^2,
\]  
(2-17)

where \( C(\omega) \) is the Fourier transform of the amplitude \( f(t) \)

\[
C(\omega) = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(t) dt.
\]  
(2-18)

Since each atom emits light for only a short time, the light from an ensemble is not monochromatic. It is physically reasonable to assume that \( f(t) \) for one atom has the exponentially decaying form

\[
f(t) = \begin{cases} 
0 & t < 0 \\
\sqrt{2\gamma} e^{i\omega t} e^{-\gamma t} & t > 0 
\end{cases}
\]  
(2-19)
which satisfies the normalization condition

\[ \int_{-\infty}^{\infty} |f(t)|^2 dt = 1 , \quad (2-20) \]

and has the Fourier components

\[ C(\omega) = \sqrt{\frac{\gamma}{\pi}} \frac{-1}{\omega_0 - \omega + i\gamma} , \quad (2-21) \]

leading to the Lorentz or dispersion profile

\[ I(\omega) = |C(\omega)|^2 = \frac{\gamma}{\pi} \frac{1}{(\omega_0 - \omega)^2 + \gamma^2} . \quad (2-22) \]

The half-half width \( \gamma \), the frequency separation at which the intensity is half the maximum, is given by the sum of the transition rates for transitions originating from either the upper or lower state of the line\textsuperscript{13}

\[ \gamma_{\ell, u} = \sum_u A_{u', u} + \sum_{\ell'} A_{\ell', \ell} . \quad (2-23) \]

Since atomic excited states have relatively long lifetimes (\( A_{u} < 10^9 \text{ sec}^{-1} \)), this natural broadening is almost always smaller (\( \Delta \lambda < 10^{-4} \lambda \)) than the other effects we will discuss. It can of course be derived rigorously from the quantum theory of radiation.\textsuperscript{25}

When the energy levels of the radiating atoms are well separated, compared to mean thermal energies, electron collisions rarely exchange energy with the radiator, but change the polarization or phase of the emitted light. Although this approximation does not hold, for example, for neutral helium\textsuperscript{7,13} (where there are nearby perturbing levels with the same \( n \) but different \( \ell \)), it is well satisfied for hydrogenic atoms. Assuming the light to be monochromatic between collisions, we have a sinusoidal wave train of duration \( \ell \), with the Fourier components
producing the intensity

\[ I_\tau(\omega) = \frac{\sin^2 \left( \frac{1}{2} (\omega_0 - \omega) \tau \right)}{2\pi \left( \frac{1}{2} (\omega_0 - \omega) \right)^2} . \]  

(2-25)

If the probability per unit time \( \gamma_c \) of a collision is constant, the intervals between collisions have the Poisson distribution

\[ P(\tau) = \gamma_c e^{-\gamma_c \tau} . \]  

(2-26)

Weighting the intensities (2-25) by the corresponding probabilities, we again arrive at the dispersion profile (2-22), now with width \( \gamma_c \).

The frequency of light emitted by a moving atom is Doppler-shifted according to

\[ \omega = \omega_0 \sqrt{1 - \frac{v_\parallel}{c} \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \left( 1 - \frac{v_\parallel}{c} \right)} . \]  

(2-27)

Assuming the atoms have a Maxwellian distribution of velocities,

\[ f_M(v) d^3v = \left( \frac{m_1}{2\pi kT_1} \right)^{3/2} \exp \left( -\frac{m_1 v^2}{2kT_1} \right) d^3v , \]  

(2-28)

the collection will emit light with the Doppler or Gaussian line profile

\[ I_D(\omega) = \frac{1}{\Delta \omega_D} \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{(\omega_0 - \omega)^2}{2\Delta \omega_D^2} \right) , \]  

(2-29)

where the characteristic width is

\[ \Delta \omega_D = \frac{\left( \frac{1}{m_1 c^2} \right)^{1/2}}{\sqrt{4\pi}} \]  

(2-30)

and the Doppler half-half width is \( \sqrt{\ln 4} \Delta \omega_D \).
In contrast to the fast electron impacts, nearby ions can usually be considered stationary, and supply only perturbing electric fields. These fields perturb the energy levels (each labeled by n, L, S, and J) of the radiating atom and usually split them into several sublevels, each a linear combination of states of different magnetic quantum number \( m_J \). Transitions between such sublevels of different principal quantum number give rise to the Stark components of a line. Since the operator \(-q_e \mathbf{E} \cdot \mathbf{r}_e\), expressing the interaction of the electric field and a given electron, has odd parity (therefore no diagonal elements), there is usually no first-order interaction, and second-order perturbation theory is used. In the hydrogenic case, however, the terms (labeled only by n) are degenerate, and a linear effect is found. This problem is most conveniently solved in the parabolic coordinates \((\xi, \eta, \phi)\):

\[
\begin{align*}
\xi &= r + z \\
\eta &= r - z \\
\tan \phi &= \frac{y}{x} \\
\left( r^2 = x^2 + y^2 + z^2 \right),
\end{align*}
\]

where the unperturbed wavefunction is

\[
\psi(n_1n_2m|\xi\eta\phi) = e^{-\frac{\xi+n}{2n}} \frac{\xi^{m/2}}{\eta^{m/2}} u_{n_1}(\xi)u_{n_2}(\eta) \frac{e^{im\phi}}{\sqrt{2\pi}}
\]

\[
\begin{align*}
n &= n_1 + n_2 + |m| + 1 = 1, 2, \ldots \\
m &= 0, \pm 1, \ldots, \pm(n-1),
\end{align*}
\]

and the energy, correct to second order in field strength, is

\[
(\text{in units of } \frac{me^4}{\hbar^2})
\]
\[ c(n_1n_2m,F) = - \frac{1}{2} \frac{Z^2}{n^2} + \frac{3}{2} \frac{n(n_1-n_2)}{Z} |F| \]
\[ - \frac{1}{16} \frac{n^4}{Z^4} [17n^2 - 3(n_1-n_2)^2 - 9m^2 + 19] |F|^2 \]

(2-33)

For a first approximation, we may assume the ions in the plasma are uncorrelated. In this case, they produce an electric field \( F \) with the Holtsmark distribution

\[ H\left(\frac{F}{F_0}\right) = \frac{2}{\pi} \frac{F}{F_0} \int_0^\infty \exp(-x^{3/2}) \sin\left(\frac{x}{F_0} F\right) x \, dx , \]

(2-34)

plotted in Fig. 2-4, where the Holtsmark normal field strength produced by perturbers with density \( N_p \) and charge \( q_p \) is

\[ F_0 = 2\pi \left( \frac{4}{15} N_p \right)^{2/3} q_p \]

(2-35)

Integrating the energies (2-33) over the distributions (2-34) for each level (though the effects on the upper level usually predominate) we arrive at the Holtsmark profile, shown for the hydrogen line \( H_B \) in Fig. 2-5. Profiles of lines subject to the linear Stark effect are usually expressed in terms of the reduced wavelength separation, defined by

\[ \alpha = \frac{\Delta \lambda}{F_0} . \]

(2-36)

Note that where there is no unshifted Stark component (as in hydrogen transitions \( n=4\rightarrow2 \) or \( 3\rightarrow1 \)), the low probability of very small fields (since \( H(0) = H'(0) = 0 \)) gives a line profile with a central dip, usually partly filled by other effects.

Finally, observed profiles are broadened by the instrument response function of the observing monochromator. According to physical optics,
Fig. 2-4 Holtsmark field strength distribution
Fig. 2-5: Holtsmark profile for the $H_S$ line
(broadened only by statistically uncorrelated ions)
it is a profile like (2-29) folded with the two rectangular slit functions, plus a constant background. With wide slits, Gaussian or triangular profiles are good approximations.

The profile of a line broadened by two independent effects is the convolution of the two profiles,

\[ I(x) = I_1(x) \otimes I_2(x) = \int_{-\infty}^{\infty} I_1(x')I_2(x'-x)dx' \]  

(2-37)

and if we assume all of these effects are independent, we may find our theoretical profile by convolving all the profiles:

\[ I_{\text{theory}} = I_{\text{natural}} \otimes I_{\text{electron}} \otimes I_{\text{Doppler}} \otimes I_{\text{ion}} \otimes I_{\text{instrument}} \]  

(2-38)

This assumption of statistical independence is reasonable for plasmas, because, e.g., collisions leading to significant changes of radiator velocities (Doppler effect) usually involve ions whose direct contribution (Stark effect) is insensitive to ion and radiator velocities.

E. Validity of LTE

A plasma is in local thermal equilibrium (LTE) if, locally and instantaneously, all quantum state population densities (except for photon states) correspond to a system in complete thermal equilibrium (CTE) which has the same mass density, energy density, and chemical composition. Departures from LTE occur when some transitions have unbalanced rates, so that some (generally low-energy) states are over- or under-populated when compared to the corresponding CTE system. In optically thin plasmas, where the rates of radiative excitation (photoexcitation and photoionization) are negligible compared to
those of radiative de-excitation (spontaneous emission and radiative recombination), the lower-energy states will be overpopulated unless collisional processes dominate radiative ones. That is, populations will be within ~10% of LTE if collisional processes are about an order of magnitude more important than radiative ones. Since collision cross sections are generally larger, and energy gaps smaller, for excited states, LTE is most easily satisfied for them. An estimate of the electron density required for the hydrogenic level \( n \) to be within ~10% of LTE with respect to the ion density is

\[
N_e > \left( \frac{7 \cdot 10^{18} \text{ cm}^{-3}}{n^{17/2}} \right) \frac{z^2}{\kappa T_{\text{H}^+}^{1/2}} \quad (2-39)
\]

The largest gap between atomic energy levels is generally between the ground and the first excited states, so the requirements for LTE for the ground state are usually the most restrictive. Near LTE, the largest transition rates are those to and from the first excited state, and collisional rates can be expected to dominate if

\[
N_e > \left( 9 \times 10^{17} \text{ cm}^{-3} \right) \left( \frac{E_2}{E_{\text{H}^+}} \right)^3 \left( \frac{\kappa T_{\text{H}^+}}{E_{\text{H}^+}} \right)^{1/2} \quad (2-40)
\]

It often happens that the resonance line is optically thick, so that radiative de-excitation of the first excited state is balanced by photoexcitation. The resonance line profile is generally dominated by Doppler broadening (for \( N_e \) sufficiently low that electron collisions cannot maintain LTE), so its optical depth can be estimated by

\[
k_{\text{reson}}' \sim 2 \times 10^{-10} \text{ cm} f_{12} \lambda_{12} \left( \frac{A E_{\text{H}^+}}{\kappa T_{\text{H}^+}} \right)^{1/2} N_{a,1}^{z-1} \quad (2-41)
\]

where the resonance line has wavelength \( \lambda_{12} \) and absorption strength \( f_{12} \), and the atoms of interest have atomic weight \( A \) and ground state density.
If the optical depth of the resonance radiation is greater than
20, the requirement (2-40) can be relaxed by about an order of magnitude.

The validity of LTE for ionization stage populations in stationary
plasmas usually need not be checked separately, since the excited
states of a given stage are well connected with the ground state of
the next ionization stage

In transient plasmas, populations may depart from LTE if equilibrium
times are long compared to the times over which plasma parameters change.
The lowest transition rates for given stage usually involve the
collisional excitation of atoms in the ground state. Assuming hydro­
genic behavior, the equilibrium time is then estimated by

\[ T_{n^{z-1}} = \left(1.1 \times 10^7 \text{sec cm}^{-3}\right) \frac{z^3}{f_{21} N_e} \left( \frac{N^z_{a+1}}{N^z_{a+1} + N^z_{a+1}} \right) \frac{E_{z-1,a}^z}{z^2 E_H} \left( \frac{kT}{z^2 E_H} \right)^{1/2} \exp \left( \frac{E_{z-1,a}^z}{V_T} \right) \]

(2-42)

where \( E_{z-1,a}^z \) is the energy of the first excited state and the term in
brackets is the fraction of atoms or ions that must be excited into
the next ionization stage. If only partial LTE is required (i.e.,
the state with principal quantum number \( n \) is in equilibrium with higher
states) the equilibrium time is much shorter, and is estimated by

\[ T_{n^{z-1}} = \left(4.5 \times 10^7 \text{sec cm}^{-3}\right) \frac{z^3}{n^4 N_e} \left( \frac{kT}{z^2 E_H} \right)^{1/2} \exp \left( \frac{2z^2 E_H}{n^3 kT} \right). \]
CHAPTER III

EXPERIMENTAL METHOD

A. Apparatus

A. T-tube and circuit. The plasma studied in this work was produced in a T-tube similar to those developed by Kolb and used in several previous experiments at the University of Maryland and elsewhere. In this device, illustrated in Fig. 3-1, an aluminum (alloy 2024-T4) electrode was sealed into either end of the top of a T-shaped tube of high-temperature glass with inside diameter of 16 mm. This tube was filled with the test gas at a pressure near .5 Torr (70 Pascals). A current flowed across the 16 mm gap between the electrodes, ionized the gas and ohmically heated it, then returned via a backstrap above the T. The backstrap current created a transverse magnetic field in the current-carrying plasma, and pressure and Lorentz force accelerated it down the leg of the T. This luminous front traveled 12 cm down the tube at several cm/μsec and struck an adjustable reflecting plate, where some of its directed motion was converted to random thermal motion. Longer expansion tubes and higher fill pressures are required for the formation of a separated shock, but this device produced the high temperatures (3.5 eV) and electron densities (2 \times 10^{17} \text{cm}^{-3}) needed to excite ionized helium lines. The decaying plasma lasted approximately one μsec.

The circuit used appears in Fig. 3-2. The relatively modest energy needed by the tube was supplied by a .5 μF capacitor charged to 40 kV (thus storing 400 J). When charged, this capacitor was disconnected.
Fig. 3-1 T-tube schematic

Fig. 3-2 Experiment circuit diagram
from both the high voltage supply and ground, preventing discharges from either electrode to the monochromator. The high-voltage circuit was enclosed by a copper shield to reduce electromagnetic interference.

To start the discharge, the nitrogen in a two-electrode pressure switch (initially at 30 PSI above atmospheric) was released until its dielectric strength was low enough for electron cascade. Since nitrogen was used, no ozone or nitrogen oxides were formed, as in a discharge in air. The poor control over discharge timing was no problem, since the discharge itself triggered the recording system.

The measured quarter-cycle time was 0.675 μsec, indicating a total circuit inductance of 370 nH. A carbon resistor of about 0.01 Ω damped out the oscillations after two cycles.

The vacuum system is shown in Fig. 3-3. During the experiment, valve V3 was closed, while shut-off valve V1 and leak valve V2 were opened, so the test gas flowed from the inlet, through liquid nitrogen cold trap CT3, into the T-tube. It then leaked into the monochromator through entrance slit S1, and was removed by pumps DP1 and MP1. V2 was adjusted so the leak rates into and out of the T-tube balanced, and the pressure, measured by thermistor gauge G2, stayed at the desired value.

Between experimental runs, the T-tube was isolated by closing slit valve V9 and shut-off valve V1, and kept clean by the small diffusion pump DP2. Cold trap CT2 was cooled by a conventional refrigeration system and valves V3 and V4 were solenoid-controlled, so this secondary pumping system could operate unattended. Since the small pump was not forced to pump through a slit, it proved more effective than the large pump at outgassing the T-tube and associated plumbing.
Fig. 3-3 Schematic of vacuum system
A.2 VUV monochromator and detector. The optical arrangement is shown in Fig. 3-4. A McPherson 225 one-meter monochromator scanned the ultraviolet lines shot-to-shot. Its 50 μm entrance slit was flush with the wall of the T-tube, about .5 mm from the reflector. Since the plasma conditions changed sharply as the reflector was moved, the position was chosen which gave the most reproducible plasma. A 1200 lines/mm Pt-coated grating, with speed about f/13.6, focused the light onto a 30 μm exit slit, for a measured reciprocal dispersion of 8.3 Å/mm (4.2 Å/mm in second order) and an approximately Gaussian instrument response function of width ν.41 Å (ν.19 Å in second order). The light then fell on a p-terphenyl coated disc, causing it to fluoresce. These visible photons left the vacuum chamber through a quartz window and were detected by an EMI 6522 photomultiplier. For some work, a 2 mm thick MgF₂ filter was placed between the exit slit and the fluorescent screen to remove light from second order, since it transmitted 40% of the light at 1215 Å but essentially none below 1100 Å. The exit slit, screen, and PM tube were replaced by a film holder for photographic work. The instrument function and wavelength calibration were checked using a low-pressure Tanaka lamp.

A.3 Visible monochromators and detectors. For diagnosis of the plasma conditions, three Jarrell-Ash visible-light monochromators were used. One 1/2-meter focal length monochromator, with instrument width .4 Å, scanned the He II 4686 line shot-to-shot to determine the electron density (from line width) and temperature (from line: continuum ratio). The reproducibility of the plasma was monitored on each shot by two 1/2-meter instruments, one for the continuum at 4976 Å.
Fig. 3-4 Schematic of optical arrangement
(sensitive to electron density), and one for the He II 4686 line (sensitive to temperature, and used for later data processing).

PM tube response was checked using neutral density filters and pulses from a light emitting diode, and was found linear for signals of up to .2 V (1.1 mA) with a PM supply voltage of 900 V.

Each PM tube housing was insulated from its monochromator, and signals were taken from both the anode (negative pulse) and last dynode (positive pulse), carried by shielded, coaxial cables terminated by 90 Ω resistors, subtracted to suppress noise, amplified, digitized, and stored electronically. For details on the waveform recorder, see Appendix A.

B. Data Reduction

The best-fit values of the four parameters (line intensity I, line position λ0, background intensity B, and electron density N_e) are found using the following procedure. Assume we have the n measurements y_1(λ_1) and the corresponding theoretical intensities T_1 = \frac{1}{F_0} T\left(\frac{\lambda_1 - \lambda_0}{F_0}\right), where T(\alpha) is the theoretical profile after convolution with the instrument profile G(\alpha)

\[ T(\alpha) = \int_{-\infty}^{\infty} S(\alpha - \alpha') G(\alpha') d\alpha', \quad (3-1) \]

and the instrument function has been transformed into \alpha-space. The best-fit values minimize the sum

\[ \sigma^2 = \frac{1}{n-4} \sum_{i=1}^{n} \left[ y_1 - (IT_1 + B) \right]^2, \quad (3-2) \]

giving the conditions
\[ \frac{\partial}{\partial I} \sigma^2 = \frac{\partial}{\partial B} \sigma^2 = 0 , \]

so I and B are found by solving the linear system

\[
\begin{pmatrix}
\sum T_1^2 & \sum T_1 \\
\sum T_1 & n
\end{pmatrix}
\begin{pmatrix}
I \\
B
\end{pmatrix} = 
\begin{pmatrix}
\sum y_i T_1 \\
\sum y_i
\end{pmatrix}.
\]  \hspace{1cm} (3-3)

The computer program "guesses" an electron density to use for the
transforming of the instrument function, convolves the theoretical and
instrument profiles, then finds \( \sigma^2 \) from (3-2) (subject to (3-3)) for
many values of \( N_e \) and \( \lambda_0 \). When the best values are found, the new \( N_e \)
is used to again transform the instrument function. The entire convolution
and fit are repeated until successive values of \( N_e \) are sufficiently close,
e.g., within 2% of each other. A general discussion of least-square fitting
when the functional parameters do not occur linearly (e.g., \( \lambda_0 \) and \( N_e \))
appears as Appendix B. Details on the computer programs appear in
Appendix C.
CHAPTER IV

RESULTS AND DISCUSSION

A. Results

Examples of photoelectric measurements of the emission profiles of the ionized helium lines at 4686, 1640 and 1215 Å are shown in Figs. 4-1 through 4-3. In each case, the solid line is the best-fit theoretical curve of Kepple,9,10 convolved with the instrument profile (taken to be Gaussian), Dashed lines are the best-fit continuum levels, determined primarily by points far from line center, which are not shown. Crosses represent points not used in the best-fit procedure.

The 4686 line was found to be unshifted, as in previous experiments.2 Its profile was in good agreement with theory, and the plasma electron density and temperature were deduced from its width and line-continuum ratio, respectively.

The position of the 1640 line was measured relative to the Al II 1670 line, and a fairly constant red shift of 0.11 Å was found. These shift measurements can be found in Table 4-1 and Fig. 4-4.

No conclusions could be drawn about the Stark width of this helium line, because the observed profile was dominated by instrument broadening.

The relative positions of the He II 1215 and Si III 1210 lines were measured photoelectrically. The helium line was found to have a red shift of approximately 0.19 Å, increasing as the density and temperature fell at the end of the discharge. The halfwidth of the 1215 line was also determined as a part of the best-fit procedure.
Fig. 4-1 Measured and best-fit profile for He II $\lambda$ 4686 Å line
Fig. 4-2 Measured and best-fit profile for He II λ 4686 line
Fig. 4-3 Measured and best-fit profile for He II $\lambda 1215$ line
Fig. 4-4 Estimated and measured shifts of He II λ 1640 Å line
<table>
<thead>
<tr>
<th></th>
<th>t</th>
<th>V-monitor</th>
<th>kT</th>
<th>N_e</th>
<th>( \lambda_{AI} )</th>
<th>( \lambda_{He} )</th>
<th>( \Delta \lambda )</th>
<th>( \Delta \lambda/N_e )</th>
</tr>
</thead>
<tbody>
<tr>
<td>unshifted</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Run 101</td>
<td>3.938</td>
<td>28.6</td>
<td>3.52±0.09</td>
<td>1.83±0.05</td>
<td>1669.52±0.01</td>
<td>1639.17±0.01</td>
<td>.11±.01</td>
<td>.060±.005</td>
</tr>
<tr>
<td></td>
<td>4.028</td>
<td>24.3</td>
<td>3.48±0.09</td>
<td>1.67±0.05</td>
<td>1669.54±0.01</td>
<td>1639.18±0.01</td>
<td>.11±.01</td>
<td>.066±.006</td>
</tr>
<tr>
<td></td>
<td>4.104</td>
<td>20.6</td>
<td>3.32±0.07</td>
<td>1.35±0.05</td>
<td>1669.54±0.02</td>
<td>1639.19±0.01</td>
<td>.12±.02</td>
<td>.089±.015</td>
</tr>
<tr>
<td>Run 99</td>
<td>3.912</td>
<td>54.3</td>
<td>3.69±0.33</td>
<td>1.42±0.04</td>
<td>1670.32±0.08</td>
<td>1639.98±0.02</td>
<td>.13±.08</td>
<td>.09±.06</td>
</tr>
<tr>
<td></td>
<td>4.004</td>
<td>46.1</td>
<td>3.42±0.12</td>
<td>1.20±0.03</td>
<td>1670.30±0.08</td>
<td>1639.97±0.02</td>
<td>.14±.08</td>
<td>.12±.07</td>
</tr>
<tr>
<td></td>
<td>4.089</td>
<td>39.2</td>
<td>3.27±0.07</td>
<td>1.02±0.03</td>
<td>1670.31±0.05</td>
<td>1640.00±0.02</td>
<td>.16±.05</td>
<td>.16±.05</td>
</tr>
<tr>
<td></td>
<td>4.146</td>
<td>33.3</td>
<td>3.19±0.07</td>
<td>.94±.03</td>
<td>1670.32±0.07</td>
<td>1639.99±0.02</td>
<td>.14±.07</td>
<td>.15±.07</td>
</tr>
</tbody>
</table>

Table 4-1 Plasma Conditions, Shifts of HeII \( \lambda 1640 \ \AA \)
These data are shown in Fig. 4-5 and Table 4-2.

B. Discussion of Possible Errors

B.1 Impurity Lines. Photographs of spectra near each of the helium lines showed many Si, O, and Al lines. The Jarrell-Ash 1/2-m monochromator could easily resolve the Si III and O II lines near He II 4686, and photoelectric scans were made using points between these impurity lines (see Fig. 4-6).

A survey spectrum was taken near the 1640 line using Kodak SWR film in the camera attachment for the McPherson 225 vacuum monochromator (see Fig. 4-7). Many Si, O, and Al lines were identified, in both first and second orders. Fortunately, none of these obscured the 1640 line. The nearby Al II 1670 line, chosen as the wavelength standard for position measurements of the 1640 line, was partially obscured by second order lines of O II and O III. Photographs using an MgF₂ filter were then taken, which showed no further problems with impurity lines. To eliminate second order lines during photoelectric scans, the filter was placed between the exit slit and the scintillating disc.

A photographic spectrum near 1215 Å showed many O II, O III, O IV Si III, and Si IV lines, including the second order O IV 608 line on the red wing of the helium line (see Fig 4-8) To eliminate these, the MgF₂ filter was again used for both photographic and photoelectric runs.

The resonance lines of N II at 1084 Å prevented any observation of the next member of the He series, while the He II 1025 line proved too weak for reliable observation.
Fig. 4-5 Estimated and measured shifts of He II λ 1215 Å line.
<table>
<thead>
<tr>
<th>t [μsec]</th>
<th>kT [eV]</th>
<th>( \lambda_{HHW, 4686}^{\text{exp}} [\text{Å}] )</th>
<th>( N_e^{HHW, 1215} [10^{17} \text{cm}^{-3}] )</th>
<th>( \lambda_{HHW, 1215}^{\text{theory}} [\text{Å}] )</th>
<th>( \lambda_{HHW, 1215}^{\text{exp}} [\text{Å}] )</th>
<th>( \lambda_{HHW, 1215}^{\text{exp}} / \lambda_{HHW, 1215}^{\text{theory}} ) [Å]</th>
<th>( \Delta \lambda [\text{Å}] )</th>
<th>( \Delta \lambda / N_e [\text{Å} / 10^{17} \text{cm}^{-3}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.864</td>
<td>2.23±.07</td>
<td>4.61±.12</td>
<td>2.23± 07</td>
<td>1.97±.05</td>
<td>2.06±.09</td>
<td>1.05±.05</td>
<td>.14±.09</td>
<td>.063±.041</td>
</tr>
<tr>
<td>3.948</td>
<td>1.93±.05</td>
<td>4 09±.09</td>
<td>1.93±.05</td>
<td>1.75±.03</td>
<td>1.96±.06</td>
<td>1.12±.04</td>
<td>.21±.04</td>
<td>.109±.021</td>
</tr>
<tr>
<td>4 040</td>
<td>1.77±.05</td>
<td>3.80±.09</td>
<td>1.77±.05</td>
<td>1.63±.03</td>
<td>1.95±.05</td>
<td>1.20±.04</td>
<td>.19±.04</td>
<td>.107±.023</td>
</tr>
<tr>
<td>4.122</td>
<td>1.66±.05</td>
<td>3.60±.09</td>
<td>1.66± 05</td>
<td>1.54±.04</td>
<td>1.88±.06</td>
<td>1.22±.05</td>
<td>.18±.04</td>
<td>.108±.024</td>
</tr>
<tr>
<td>4.191</td>
<td>1.62±.06</td>
<td>3.53±.11</td>
<td>1.62±.06</td>
<td>1.51±.05</td>
<td>1.88±.06</td>
<td>1.25±.06</td>
<td>.19±.04</td>
<td>.117±.052</td>
</tr>
<tr>
<td>4.245</td>
<td>1.46±.07</td>
<td>3.24±.13</td>
<td>1.46±.07</td>
<td>1.38±.06</td>
<td>1.82±.05</td>
<td>1.32±.07</td>
<td>.27±.04</td>
<td>.185±.027</td>
</tr>
</tbody>
</table>

Table 4-2 Plasma Conditions, Shifts and Widths of HeII \( \lambda 1215 \) Å
Fig. 4-6 Densitometer scan of spectrum near He II \( \lambda \) 4686 Å line
Fig. 4-7 Densitometer scan of spectrum near He II λ 1640.8 line.

- Al III 1605
- Al III 1612
- Si IV 815
- Si IV 818
- He II 1640.48
- O III 1660.80 + O IV 830.51
- O IV 831.07
- O III 833.33
- O III 833.74
- O II 834.46
- Al II 1670.79 + O III 835
Fig. 4-8 Densitometer scan of spectrum near He II λ 1215 Å line
B.2 Wavelength Standards. All line position measurements were made relative to nearby impurity lines, and the accuracy of this procedure had to be verified. The Stark shifts of these ion lines are expected to be small\(^4\) (just as their widths are small), but a plasma polarization shift certainly cannot be ruled out a priori. To check for such shifts, several line position measurements were made on a Grant comparator-microphotometer. The second-order lines were found to be shifted with respect to the first-order lines by \(0.10\ \AA\), but otherwise, shifts were less than the measurement accuracy of \(0.05\ \AA\). This is consistent with previous measurements,\(^3\) in which no shifts were found for the \(\text{O III}\) and \(\text{N III}\) lines near \(300\ \AA\). In photoelectric (time-resolved) studies, no absolute shifts of the reference lines were measured as the plasma cooled, also arguing against substantial absolute shifts. Only the statistical errors in the measured shifts are indicated in the tables and figures.

The monochromator wavelength scale was checked by measuring photographically the wavelength displacement between settings corresponding to the centers of the helium and reference lines. The errors in both cases were less than the setting error of \(0.02\ \AA\).

B.3 \(\text{He II 1215 Asymmetry.}\) The helium 1215 line was expected to have a symmetric, double-peak profile (like that of \(\text{H}_\beta\)), but photoelectric scans showed only the peak on the blue side (see Fig 4-3). This was interpreted as showing reabsorption by hydrogen in a cooler boundary layer, since the hydrogen Lyman-\(\alpha\) line lies \(0.50\ \AA\) to the red of the (unshifted) helium line center. To check this explanation, two scans were made, using mixtures of helium plus 0.5% hydrogen, and helium plus 1.0% deuterium, respectively. The amount of absorption increased with the increasing admixture of hydrogen, and, in the case of the deuterium, the dip shifted to the blue, as expected.
The residual concentration of hydrogen was estimated from these runs to be approximately 0.2%. Since natural, Doppler, and Stark broadening are all very small for the hydrogen line (<1 Å), points near the dip were merely excluded from the fitting procedure.

B.4 Departure from LTE. Temperature determination from a helium ion line: continuum ratio requires that LTE holds also for the ion ground state populations, so that the line intensity (proportional to the population in the excited state) and the continuum intensity (due mainly to recombination radiation) both have their equilibrium values. The equilibration time for atomic states can be estimated from (2-42) to be only a few nanoseconds, for both neutral and ionized helium. On the other hand, the recombination times (into the ground states) are estimated to be \(2\ \mu\text{sec}\) for formation of singly ionized helium and \(20\ \mu\text{sec}\) for neutral helium. Singly and doubly ionized states are, then, expected to be overpopulated, simulating a temperature higher than the true electron temperature.

For the validity of complete LTE in a stationary plasma with temperatures near those in the experiment, Eq. (2-11) gives an optical depth of \(\simeq 150\), for the resonance line (He II \(\lambda 304\ Å\)). We are thus justified in relaxing (2-40) by an order of magnitude, and the electron density required for complete LTE is \(N_e \simeq 1.4 \times 10^{18}\ \text{cm}^{-3}\), which is not reached in the experiment. On the other hand, the requirement (2-39) for partial LTE for the level \(n=4\) (upper state of the 4686 Å line) is easily satisfied.

Since the actual electron density is about an order of magnitude lower than that required for complete LTE, and the continuum intensity is proportional to the electron density while the line intensity is not, we estimate that the line:continuum ratio may be too high by an order of magnitude, compared with the LTE value at the true
temperature. This yields a temperature (≈3.5 eV) that is too high by about .5 eV. Similarly, if the neutral excited state population density were too low by an order of magnitude, the intensity ratio of an ionized and a neutral line would overestimate the temperature by about .5 eV. A measurement of the intensity ratio of the He II 4686 and the He I 3889 lines was performed, yielding temperatures near 4.1 eV. Since the two effects (overpopulation of singly ionized states due to recombination relaxation during the rapid cooling, and overpopulation of excited states of He II due to low collision rates) are additive, the true electron temperature is estimated to be less than the lower figure by ≈20%, i.e., near 3.0 eV.

A previous measurement of the absolute intensity of the He II 4686 line in a shock-tube plasma at $N_e \approx 10^{17}$ cm$^{-3}$ indicated the populations of the lower excited states of the ion deviate by perhaps a factor of 4 from LTE. However, measurements of temperature in the same experiment by Thompson scattering of laser light (which does not depend on LTE for atomic states) and the intensity ratios of the He II 4686 and He I 5876 lines showed good agreement.

B.5 Summary of Errors. Possible errors in the determination of electron density were judged to be 5% due to statistical fluctuations and 10-15% due to theoretical uncertainties. Errors in temperature measurements were estimated to be .1 eV statistical and .2 eV theoretical (after applying the 20% correction). These possible diagnostic errors were not judged to endanger the principal conclusions of the work. The tables and figures indicate only statistical errors.

Errors in the measurements of the shifts were .05 Å or less due to statistical fluctuations. Systematic errors due to the shift of the
reference lines could not be ruled out, but were shown to be less than .05 Å and are expected to be smaller.

C. Discussion of Results

As mentioned in the Introduction (Chapter I), previous shift measurements of He ion lines have concentrated on the Lyman-series lines \( n_{\text{lower}} = 1 \). In principle, these measurements can be used to calculate the energy level perturbations, and the shifts of the "Balmer"-series lines can be found in turn. Since the agreement between the various measurements is so poor, little is learned in this way.

The polarization shift is difficult to treat theoretically, and only estimates have been made thus far. Conceptually, the radiating ion is expected to attract plasma electrons, which partially screen the nuclear charge seen by the optical electron. A simple classical argument gives the wavelength (or wavenumber) shifts of the Lyman-series lines to be

\[
\frac{\Delta \lambda}{\lambda_0} = \Delta \nu = - \frac{8}{3} \pi \frac{N e^2}{a_0^2} n^2 (n^2 + 1) \exp \left( \frac{V}{kT} \right),
\]

where \( a_0 \) is the radius of the first Bohr orbit: \( a_0 = \hbar^2/ma^2 \), and \( V \) is the interaction energy between the perturbing plasma electron and the radiating ion. Since the wave packet of the perturbing electron will be comparable in size to the atom, Griem proposes to use the averaged interaction \( V = e^2/r \), where \( r \) is the characteristic distance between the nucleus and the optical electron. \( r = n^2 a_0/z \). Neiger proposes the modified formula \( V = (1/2)e^2/r \), which is the electrostatic energy of a uniform sphere of charge \( e \) and radius \( r \).
in the field of an equal but opposite charge at its center. Burgess and Peacock argue that the density of electrons near an ion is low enough that their velocities are not in equilibrium with the surrounding plasma, being directly related to their electrostatic energies. They suggest using the interaction energy at the average perturber-perturber distance, $V = \frac{2.1/3}{n_e}$. Note that all these estimates predict blue shifts (for the Lyman-series lines) proportional to $n_e$, but decreasing with temperature (since, at high temperature, the electron's thermal energy is large compared with the electron-ion interaction energy, and it doesn't see the potential well). Denoting by $V_n$ the chosen interaction energy when the optical electron has principal quantum number $n$, and expressing the unperturbed energy levels in terms of the Rydberg constant $R$, we find, for the wavenumber shifts of the "Balmer"-series lines,

$$\Delta \nu = \frac{8}{3} \pi \frac{a_0^3}{z^2} R \left\{ (n^4-1)\exp \left( \frac{V_n}{\kappa T} \right) - (2^4-1)\exp \left( \frac{V_2}{\kappa T} \right) \right\}.$$  

This can be converted to a wavelength shift by multiplying with $\lambda_0^2$, or an energy shift by multiplying by $hc$. Shifts predicted by each of these choices for $V$ ($ze^2/n^2a_0$, 3/2 $ze^2/n^2a_0$, and $e^2n_e^{1/3}$) are plotted in Figs 4-4 and 4-5. For both lines, Burgess and Peacock predict very small blue shifts, nearly independent of temperature. Griem's estimate gives somewhat larger shifts, while the stronger interaction proposed by Neiger gives large shifts with strong temperature dependence. Using the measured values of the temperature, the data are consistent with an interaction energy between those of Griem and Neiger, while Burgess and Peacock underestimate the shifts. To illustrate the effect of the systematic error discussed above in the temperature
measurement, the shift predicted by Griem's formula was recalculated using a 20% lower temperature, the results being shown as the dashed curve in Figs. 4-4 and 4-5. After this correction, his interaction energy gives the best fit to the data.

The halfwidth of the 1215 Å line was up to 30% greater than that calculated by Kepple. This is to be compared to a previous theta-pinch experiment, in which the ratio of the widths of the 4686 and 1215 Å lines agreed with the calculated value. However, this experiment was done at a substantially higher temperature, $T_e > 10$ eV, so that the difference may not be significant.

D. Conclusions and Suggestions

Shifts have been measured of the first two lines of the "Balmer" series of ionized helium. They are consistent with a plasma polarization shift, where the interaction energy between the radiating ion and the plasma electrons is between those proposed by Griem and Neiger and probably closer to the former.

The Stark width of the 1215 Å line of ionized helium has been measured, and found to be up to 30% greater than calculated by Kepple, and increasing as the temperature and density of the plasma decreased at the end of the discharge. This is perhaps due to an increased interference by the 1215 Å line of hydrogen.

Further studies of the plasma polarization shift might include more careful measurements of shifts of the hydrogenic spectra of heavier atoms, e.g., C VI 33.8 Å. Previous measurements showed no shifts, but with a possible error of .05 Å. (In this connection, it is interesting to note that measured center wavelengths, e.g.,
of helium-like copper (Cu XXVIII) are slightly below theoretically predicted values.) An attempt might also be made to observe shifts of the higher "Balmer"-series members of ionized helium, perhaps in a Z pinch or θ pinch, with their greater optical depth.
APPENDIX A

WAVEFORM RECORDER

To reduce the error and delay of manual data taking with the usual Polaroid oscillographs, a waveform recorder was designed and built for this experiment (Fig. A-1). The signal from one of the PM tubes is amplified and applied simultaneously to 31 comparators. A voltage divider provides reference voltages for the comparators, so for a given signal voltage some of the comparators will be "on" and the rest "off". Integrated circuits accept the output of all the comparators, count the number "on", calculate the corresponding 5-bit binary number, and store it in a 5 bit by 64 word random access memory. When triggered, control circuits advance the memory address counter and give write commands once every 100 nanoseconds (or selectable, slower rates) for a total of 64 cycles. It then switches to "playback" mode, supplying the stored numbers, each in turn, to a digital-to-analog converter. This analog signal is a reconstructed version of the original signal, and can be displayed on an oscilloscope.

The recorder consists of five such analog-to-digital converters and memories, plus two digital-to-analog converters, so 5 signals can be recorded, then any two displayed simultaneously.

If the waveform is acceptable, the investigator may set the twelve "fixed data" thumbwheel switches and initiate recording. The shot number (incremented each time the device is triggered), the fixed data, and the contents of all 5 digital memories are written to a 9-track magnetic tape for later computer processing. The waveform recorder then
Fig. A-1 Block diagram of waveform recorder
reverts to "ready" mode, waiting for the next trigger pulse. If the shot was unacceptable (due to switch misfire or abnormal time history of a monitor signal, for example), recording can be bypassed.

Details on operation procedures and performance specifications of the waveform recorder appear in the following instruction sheet.
1. General Information

The Digital Data Acquisition System (DDAS) is a high speed analog to digital converter and memory. It can record 64 data samples on each of 5 channels, with a sample interval as short as 100 nsec. These stored samples can be displayed on an oscilloscope and recorded onto a 9-track magnetic tape.

2. Technical Specifications

- Sample rate, once every: 0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10.0, or 20.0 μsec.
- Internal amplifier risetime: 80 nsec
- Useful signal range: 0 to +32 V
- Maximum signal range: -1 to +1 V
- Resolution: 3.1% of full scale
- Channels: 5
- Signal input impedance: 50 Ω
- Trigger level: +1.1 V
- Maximum trigger signal range: -0.6 to +5 V
- Trigger input impedance: 1MΩ
- Playback sweep output: 22.7 Hz sawtooth, 0-2.6 V
- Analog output: 0-5 V
- Enabling circuit: enabled if external circuit resistance is less than 100 Ω
- Mating input amplifier: Tektronix type 127 preamp power supply, with matching Tektronix oscilloscope preamp.
- Mating digital tape deck: Cipher model 70M-360, producing 800 BPI, 9-track, IBM-compatible magnetic tapes.
- Magnetic tape record: 329 bytes of 8 bits each...
  - 6 bytes (BCD, 2 digits/byte) fixed data from thumbwheel switches
  - 3 bytes (BCD, 4 low order bits) experiment count
  - 320 bytes (binary, 5 low order bits) data, grouped by time
3. Installation

For optimum protection against radio frequency interference, the unit should be mounted in a shielded 19 in. relay rack. Several inches clearance below the unit are necessary for ventilation.

4. Operation

The Cipher tape deck should never be switched on unless the DDAS is on, so the proper logic inputs are provided.

1. Turn on the DDAS and associated preamplifiers. Allow preamps to warm up.

2. If a tape is desired, turn the tape deck on and load a tape. The "RECORER READY" lamp should light.

3. Switch the operating mode to "AUTO SEQUENCE", switch to "TRIGGER ENABLE INT", and press "RECORD BYPASS". The "ENABLED" lamp should light.

4. Switch "DISPLAY CHANNEL SELECT" to "1". The "A-D DISPLAY" lamps are now displaying, in binary digital form, the signal on channel 1.

5. Ground the channel 1 preamp input. Advance the preamp "vertical position" control until all display lamps are lit. If this cannot be done, adjust the 127 preamp power supply "DC level" (on top of case).

6. Back off the "vertical position" control until all lamps just go out. The zero level is now adjusted. Repeat steps 4-6 for the remaining channels now, and frequently during the experiment.

7. Connect the trigger and signal cables. If an "enable" circuit cable is to be used, connect it and switch to "TRIGGER ENABLE EXT". Set the desired sampling interval. When triggered (by a signal or by using the "MAN TRIGGER" button) the unit will record its 64 samples of each channel and increment the "EXPERIMENT COUNT".

8. If a visual monitor is desired, connect the "PLAYBACK SWEEP" to the "EXT HORIZ IN" jack of an oscilloscope, and one or both of the "ANALOG OUTPUT"'s to the vertical amplifier inputs. Set "ANALOG CHAN SELECT" to the desired channels.

9. When a signal is recorded, the unit will automatically switch to playback mode, the corresponding mode lamp will light, and the stored waveforms will be displayed on the oscilloscope.
10. If a recording is desired, set the desired "FIXED DATA", and press "RECORD DATA". Otherwise, press "RECORD BYPASS". The unit is again ready to record a set of signals. The unit may be switched to "MAN PLAYBACK" to again display the recorded signals.

11. After experiment has been completed, press "EOF" several times, and rewind and unload the tape.

12. Turn the tape deck off, then the DDAS and other equipment.

Alternate operating modes are provided for diagnostic purposes. In "SINGLE STEP PLAYBACK" mode, the contents of one word in memory, corresponding to the "DISPLAY CHANNEL SELECT" setting and the octal address shown under "MEMORY ADDRESS", are displayed under "MEMORY DISPLAY" and appear at the "ANALOG OUTPUT" jacks. The associated pushbutton steps to the next sample.

In "MAN SAMPLE" mode, the unit stores samples one at a time, when the "SAMPLE STROBE" pushbutton is pressed. The unit must be enabled and triggered before sampling can begin.

In "CAL" mode, the analog to digital converters operate continuously and any of them can be displayed on the "A-D DISPLAY" lamps.
APPENDIX B

STATISTICS

In most experiments the investigator assumes a functional form governing his data which has several parameters, and the object of his experiment is to determine the values of the parameters. If there is only one parameter, the quoted result might be

\[ a = a^* \pm \sigma, \]

where \( a \) is the true value (usually unknown), \( a^* \) is the "best" value which can be determined using the data, and \( \sigma \) indicates the error in \( a^* \). We usually mean by \( \sigma \) the mean square deviation of the data from the best value

\[ \sigma^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - a)^2, \quad (B-1) \]

where the \( x_i \) are the results from several similar experiments. It is necessary to extend this to the case of several parameters and specify a way of calculating the quoted values.

Assume the functional form is

\[ y = f(a, x), \quad (B-2) \]

where \( x \) is the independent variable, \( y \) the dependent variable, and the \( a \) are parameters. We define the error function

\[ M(a) = \sum_{k=1}^{n} \frac{(y_k - f(a, x_k))^2}{\sigma(x_k)^2}, \quad (B-3) \]

and let the "best" \( a^* \) be that value \( a^* \) which minimizes \( M \). We find it by solving the set of \( m \) equations.
\[ \frac{\partial M(\theta)}{\partial a_1} \bigg|_{\theta = \theta}^* = 0 \] (B-4)

The errors in these parameters are given by the elements of the variance-covariance matrix:

\[ \sigma_{ij} = (a_i - a_i^*)(a_j - a_j^*) \] (B-5)

which can be calculated from:

\[ \sigma_{ij} = (H^{-1})_{ij} \quad H_{ij} = \frac{1}{2} \frac{\partial^2 M(\theta)}{\partial a_i \partial a_j} \] (B-6)

The variance of one of the parameters is then \( \sigma^2 = \sigma_{11} \), and the correlation matrix is

\[ C_{1j} = \frac{\sigma_{1j}}{\sigma_{11} \sigma_{jj}^{\frac{1}{2}}} \] (B-7)

If all the \( \sigma(x_k) \) have a common value \( \sigma \), the solution of (B.4) is independent of that value. After this least square solution is found, \( \sigma \) can be calculated using

\[ \sigma^2 = \frac{1}{n-m} \sum_{k=1}^{n} [y_k - f(\theta; x_k)]^2 \] (B-8)

where we divide by \( n-m \) because after the parameters \( a_1 \ldots a_m \) have been calculated from the data, only \( n-m \) degrees of freedom remain.

If \( f(\theta; x) \) is linear in its parameters, the calculations are, of course, much simpler, since (B-4) is then a linear system which can be solved exactly. Failing this, a search must be performed in \( \theta \) space for the best value.
APPENDIX C

PROGRAMS

The data read from the waveform recorder tapes are processed by several programs, each accepting an input file plus control or data cards, and producing one or more output files. The last programs, PROFILE, VPLOT, and THEORY, also print their results. Other programs are available to read and list each file for debugging. All mainline programs were written in FORTRAN for use on a Univac 1108 computer with the EXEC-8 operating system. Intermediate files are "direct-access" files on disc or drum storage, like those developed by IBM for their computers, but not defined within ANS FORTRAN. Other nonstandard features used include PARAMETER statements and FORTRAN procedures.

The first program, REVERT, uses the assembly-language subroutine TREAD to read the 9-track tape produced by the waveform recorder. The tape record format is shown in Fig. C-1. REVERT assumes the scale settings of the input amplifiers and the sample rate of the recorder were set on the "fixed data" thumbwheel switches. The alphanumeric file header (a prose description of the run), number of channels used, and wavelength for each channel and shot number are read from cards. The file header is written into the output file, copied by later programs, and identifies all printed output. Specified shots may be dropped at this point.

Since the waveform recorder stores 6.4 μsec of the signal, while the plasma lasts only about one μsec, REVERT tries to select only the useful part of each signal. The first twelve records are read, the average time $T_{max}$ of the maximum of the monitor signal is found, and the tape is...
rewound. Each record is then read, and the data for eight samples, starting at time \( T_{\text{max}} \), are scaled and written to the output file, with format shown in Fig. C-2. An end-of-file marker is written after the last record.

During the experiment, the light is sometimes attenuated to prevent PM tube saturation, and PARAM corrects the measured intensities to account for this. Since PROFILE requires that the monitor signal be strictly decreasing, PARAM also chooses a decreasing portion of each signal and discards the rest. The output record format is shown in Fig. C-3.

BSORT sorts the records, first on wavelength, then on shot number. Experimental points can be taken in any order, but in this step all data for a given wavelength are collected. The format of the records is unchanged by BSORT.

PROFILE unfolds the data, recorded as intensity as a function of time at different wavelengths, into intensity as a function of wavelength (a line profile) at different times. Since the ionized helium line intensities are sensitive to temperature, all data for one profile must be taken under the same plasma conditions. PROFILE does this by taking all the data for equal monitor signal (from the total intensity of the He II 4686 line). The time at which the monitor signal decays to this level is found, and the shot is discarded if this time is further than 1.73 standard deviations from the mean. Similarly, any intensities at a given wavelength which differ from the mean by more than 1.8 standard deviations are discarded. Profiles are then found for successively lower monitor intensities (therefore later times). The means and standard deviations of intensities at each wavelength go to one file (shown in Fig. C-4), which VPLOT uses to make a printer-plot of the line
profile. All undeleted data points are written to a second file (shown in Fig. C-5), used for fitting.

The actual least-squares fit is done by THEORY. As described in the section on data reduction, the convolution of the theoretical line profile with the instrument response function is done first, in alpha space, using an assumed electron density. The instrument function is assumed Gaussian, so the convolution integrals are done using the Gaussian-Hermite 3-point quadrature formula. This profile is fit to the experimental data and a new electron density is found. The convolution and fit are repeated until the electron density converges, usually within four iterations. Each of these fits requires a search for the values of the four parameters (line intensity I, background intensity B, line center \( \lambda_0 \), and electron density \( N_e \) (line width)) that minimize the mean square deviation \( \sigma^2 \) of the fitting function from the experimental points. The subroutine ZXPOWL, from the International Mathematical and Statistical Library (IMSL) uses the function-minimization algorithm described by Zangwill to find the best-fit values of \( \lambda_0 \) and \( N_e \). For each trial values of \( \lambda_0 \) and \( N_e \), it calls the subroutine FUNCT3, which in turn calls other subroutines to calculate the best values of the two linear parameters, and the corresponding \( \sigma^2 \), using standard methods.

When the best values of all four parameters are found, subroutine FUNCT2 finds the second derivative matrix of \( \sigma^2 \) numerically, inverts it, and normalizes it to get the standard deviations and correlation matrix of the best-fit parameters. If the line is He II 4686, it uses the line:continuum ratio to calculate the plasma temperature Sub-
routine TPLOT plots the average of the experimental points at each wavelength, the best-fit theoretical profile, and the background level. The entire procedure is repeated for each profile, but since the line center and electron density are carried over each time, subsequent fits converge rapidly.

<table>
<thead>
<tr>
<th>6 bytes</th>
<th>3 bytes</th>
<th>320 bytes</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIXED</td>
<td>COUNT</td>
<td>DATA</td>
</tr>
</tbody>
</table>

- **FIXED**: 6 bytes BCD, 2 characters/byte, data from thumbwheel switches
- **COUNT**: 3 bytes BCD, 1 character/byte, shot number
- **DATA**: 320 bytes binary number, 1/byte, data, grouped by time

**Fig. C-1** Record format of waveform recorder tape

<table>
<thead>
<tr>
<th>2 words</th>
<th>1 word</th>
<th>1 word</th>
<th>16 words</th>
</tr>
</thead>
<tbody>
<tr>
<td>LABEL</td>
<td>SCALE</td>
<td>COUNT</td>
<td>( T_1 ), ( Y_1 ), ( T_2 ), ( Y_2 ), \ldots ( T_8 ), ( Y_8 )</td>
</tr>
</tbody>
</table>

- **LABEL**: 2 words, FIELDATA
- **SCALE**: 1 word, real (R), Amplification on preamplifier (V/div)
- **COUNT**: 1 word, integer, Shot number (same as above).
- **\( T_i \)**: 1 word, R, Time of sample (\( \mu \)sec. after trigger pulse)
- **\( Y_i \)**: 1 word, R, Signal amplitude (V)

**Fig. C-2** Format of data record written by REVERT
2 words 1 word 1 word 1 word 8 words 8 words

<table>
<thead>
<tr>
<th>LABEL</th>
<th>SCALE</th>
<th>COUNT</th>
<th>POINTS</th>
<th>$T_1T_2\ldots T_8$</th>
<th>$Y_1Y_2\ldots Y_8$</th>
</tr>
</thead>
</table>

LABEL, SCALE, COUNT, $T_1$, $Y_1$ as before

POINTS 1 word, integer Number of data points (always 8)

total: 21 words/record

Fig. C-3 Format of data record written by PARAM or BSORT

1 word 36 words 36 words 36 words

<table>
<thead>
<tr>
<th>MONITOR</th>
<th>WAVELENGTH</th>
<th>AVERAGE</th>
<th>SIGMA</th>
</tr>
</thead>
</table>

MONITOR 1 word, R Intensity of monitor for this profile

WAVELENGTH 36 words, R Wavelengths (Å)

AVERAGE 36 words, R Average of signal intensities at corresponding wavelength.

SIGMA 36 words, R Standard deviation of signal intensities

total: 109 words/record

Fig. C-4 Format of plot-file data record written by PROFILE

1 word 55 words 36 words 36 words $28 \times 36 = 1008$ words

<table>
<thead>
<tr>
<th>MONITOR</th>
<th>BLOCK</th>
<th>NUMBER</th>
<th>WAVELENGTH</th>
<th>INTENSITY</th>
</tr>
</thead>
</table>

MONITOR 1 word, R Intensity of monitor signal for this profile

BLOCK 54 words, integer (currently not used)

NUMBER 36 words, R number of shots at this wavelength

WAVELENGTH 36 words, R Wavelengths

INTENSITY 1008 words, R INTENSITY (I,J) is the signal for the Jth shot at wavelength WAVELENGTH(I)

total: 1135 words/record

Fig. C-5 Format of fit-file data record written by PROFILE.
A Note on Program Documentation

A code is used to describe the parameters of some subroutines. For example, in TIM,

```
INT R,I  Given intensity ,
```

the R indicates INT is real (single precision floating point) and the I means it's used only for input (i.e., the subroutine doesn't change its value). Possible parameter modes are:

- **F**: single precision floating point
- **DP**: double precision floating point
- **I**: integer
- **S**: statement number, for alternate return
- **L**: logical
- **C**: complex,

and possible uses are:

- **I**: input only (unchanged)
- **O**: output only (changed, contains useful information)
- **IO**: input and output
- **W**: work area (changed, not meaningful on return).
Programs Listed

REVERT

TREAD*, OPT*

PARAM

BSORT

STORES, START, SADD, SDROP, HADD, HDROP, ADDTO,
FINDTO, EPUSH, EPOP

PROFILE

TIM, INTENS, LOOKUP, YESNO*

VPLOT

THEORY

DBANK, GROUP, FETCHS, FUNCT3, FUNCT2, TPLOT,
AXISN**, NEWS, NEWT, NEWU, SIGMA, SYMSLV**, VALUE**

*Programs in UNIVAC Assembly Language.

**These programs may be of general interest
***** REVERT *****

2037JU1#OKSPACE$1.REVERT

NAME...

REVERT

PURPOSE...

TO ACCEPT A TAPE PRODUCED BY THE DIGITAL DATA ACQUISITION SYSTEM AND PRODUC E A FILE ACCEPTABLE TO PROGRAM "PARAM".

USAGE...

\texttt{SNT RTFERT (NOT \texttt{SREVERT})}

\texttt{<DATA CARDS>}

OPTIONS:

'L' PRINTS INFORMATION FROM DATA CARDS AND FIXED DATA FROM TAPE RECORDS (THUMMWHEEL SWITCHES)

'H' IGNORES IMPROPER SCALE OR INTERVAL FROM TAPE RECORD HEADER...NO MESSAGES

'B' Omit INITIAL REWIND (DEFAULT: REWIND TAPE BEFORE READING)

INPUT...

DATA TAPE WITH NAME 'INTAPE', PRODUCED BY THE DIGITAL DATA ACQUISITION SYSTEM DATA FROM THUMMWHEEL SWITCHES IS INTERPRETED AS FOLLOWS:

DIGITS 1-5...SCALE (V/DIV) FOR CHANNELS 1-5

DIGIT 6...SAMPLE INTERVAL (MICROSEC)

SETTING 0 1 2 3 4 5 6 7 8 9

MEANING LEGAL .005 .01 .02 .05 1, 2,

.005 .LE. SCALE .LE. 2.

.05 .LE. INTERVAL .LE. P.

INTERVAL SPECIFIED ON CARD 3 SUPERCEDES DIGIT 6.

A WARNING IS PRINTED IF INTERVAL ISN'T .1 MICROSEC.

THE FOLLOWING DATA CARDS:

CARDS 1 AND 2...

\texttt{(72A1/72A1) ALPHANUMERIC FILE HEADER IMAGES}

CARO 3...

\texttt{(IS) NUMBER OF CHANNELS BEING USED}

\texttt{(F9.0) SAMPLE INTERVAL IN MICROSECONDS}

\texttt{(IS) MONITOR SIGNAL CHANNEL (IF BLANK, THE PROGRAM USES THE FIRST CHANNEL WITH BLANKS IN THE WAVELENGTH SPECIFICATION COLUMNS OF CARD 4.)}

\texttt{(IS) STARTING SAMPLE NUMBER (IF BLANK, THE PROGRAM READS THE FIRST 12 RECORDS AND USES THE AVERAGE OF THE MAXIMA OF THE MONITOR.)}

CARDS 4-N

\texttt{(SORTED BY SHOT # INCREASING) FIRST SHOT NUMBER OF A GROUP OF SHOTS WITH THIS SET OF WAVELENGTH SETTINGS.}

\texttt{(5F5.1) WAVELENGTHS IN ANGSTROMS FOR EACH CHANNEL}

\texttt{BLANK FIELD INDICATES A MONITOR CHANNEL}

\texttt{CARD N+1... QEOF ' IN FIRST FIVE COLUMNS}

\texttt{CARDS N+2 - N}

\texttt{(IS) SHOT NUMBER WITH INCORRECT SCALE #}

\texttt{(S5F5.4) NEW SCALE #S (BLANKS FOR CORRECT ONES)}

\texttt{CARD M+1...}
OPEN * OF 'In first file columns'

INPUT...

DATA RECORD FORMAT: LABEL(2), SCALE, NSHOT, T1, T2, T3, T4...

TOTAL: 49 WORDS

SUBPROGRAMS REQUIRED...

BEGIN

OPT

READ

PARAMETER POINTS=10

PARAMETER MPTS=15

PARAMETER MCHAN=10

PARAMETER NCHANS=POINTS

INTEGER HEADER(10)

LOGICAL VARIED, GIVEN

LOGICAL OPT, ICHAN, IREC...

DIMENSION SCALE(9), NPTS=15

REAL IREC(NPTS)

- INREC(NPTS), HEAD(NPTS, MCHAN), LSHOT(1:BAD)

GOOD(NCHAN, MCHAN)

DATA SCALE/05, 01, 02, 03, 04,

- /RECORD(1), HEAD(1), RECORD(1)

DATA NPTS, NFILE, ENDCARD, HDR, CARD, NAME, SAVE

- / 1, 10, IEOF, 9, 5, FALSE, FALSE,

DATA 4CHAN, MPTS, SRCU, v=0,

- / MCHAN, NPTS, SRCU, HDR

COMMENT NSHOT=HUP(12)+151u(3+64)

CALL BEGIN(REVERT 1, 0, L)

QUIT=OPT(1, L)

IF(NPT=OPT) CALL ME=I.

DEFINE FILE .=FILE(F6:RECORD(1:RECORD(1))

NREC=1

TRANSFER HEADER INFORMATION

DO 10 I=1, 2

READ(CARD, 810, END=100, IHEAD)

IF(IHEADN=810, IHEAD)

READ(CARD, 810, END=100, IHEAD)

WRITE(NFILE, IHEAD, HEADER)

IF(IHEADN=810, IHEAD)

READ(CARD, 820, END=100, ICHAN=K, MCHAN=K, MONT STATES)

WRITE(NFILE, IHEAD, HEADER)

10 IHEAD=IHEAD+1

IHEAD=IHEAD+1

END

INPUT...

DATA RECORD FORMAT: LABEL(2), SCALE, NSHOT, T1, T2, T3, T4...

TOTAL: 49 WORDS

SUBPROGRAMS REQUIRED...

BEGIN

OPT

READ

PARAMETER POINTS=10

PARAMETER MPTS=15

PARAMETER MCHAN=10

PARAMETER NCHANS=POINTS

INTEGER HEADER(10)

LOGICAL VARIED, GIVEN

LOGICAL OPT, ICHAN, IREC...

DIMENSION SCALE(9), NPTS=15

REAL IREC(NPTS)

- INREC(NPTS), HEAD(NPTS, MCHAN), LSHOT(1:BAD)

GOOD(NCHAN, MCHAN)

DATA SCALE/05, 01, 02, 03, 04,

- /RECORD(1), HEAD(1), RECORD(1)

DATA NPTS, NFILE, ENDCARD, HDR, CARD, NAME, SAVE

- / 1, 10, IEOF, 9, 5, FALSE, FALSE,

DATA 4CHAN, MPTS, SRCU, v=0,

- / MCHAN, NPTS, SRCU, HDR

COMMENT NSHOT=HUP(12)+151u(3+64)

CALL BEGIN(REVERT 1, 0, L)

QUIT=OPT(1, L)

IF(NPT=OPT) CALL ME=I.

DEFINE FILE .=FILE(F6:RECORD(1:RECORD(1))

NREC=1

TRANSFER HEADER INFORMATION

DO 10 I=1, 2

READ(CARD, 810, END=100, IHEAD)

IF(IHEADN=810, IHEAD)

READ(CARD, 810, END=100, IHEAD)

WRITE(NFILE, IHEAD, HEADER)

IF(IHEADN=810, IHEAD)

READ(CARD, 820, END=100, ICHAN=K, MCHAN=K, MONT STATES)

WRITE(NFILE, IHEAD, HEADER)

10 IHEAD=IHEAD+1

IHEAD=IHEAD+1

END

ORIGINAL PAGE IS OF POOR QUALITY
****** ALGOL ******

114 IF(LUST+GT.*CHN+ OR. NILCHAN+LF.*01G) TO 138
115 IF(SAMPLE+EQ.0.) GO TO 12
117 GIVE=TRUE.
118 IF(POS+LT.+0. OR. MOJIT+GT.+NCHAN) GO TO 112
119 IF(KTIME+LT.+0. OR. KTIME+GT.+5+G. TO 114
120 IF(KTIMEPRINT+815+CHAN+5A PLEASE+MONIT+KTIME
121 815 FORMAT(1X//1X12.CHAINLS USED+:+F6.2:+USE SAMPLE INTERVAL/)
122 - ' CHANNEL+12+ IS MONITOR: STARTING CHANNEL IS'+14)
123 IF(SAMPLE+EQ.0.) GO TO 112
124 C READ WAVELENGTHS FOR EACH SHOT NUMBER
125 C 825 FORMAT(1X//10 SHOT # WAVELENGTHS/)
126 DO 23 NPTS+2+PTS
127 READ(50,830,END+25) KSHOT(NPTS), (WAVEL(NPTS+M),M=1+NCHAN)
128 830 FORMAT(15.5AN5)
129 DO 20 J=1,NCHAN
130 20 DECODE(832#AVEL(NPTS+M)N(M)
132 832 FORMAT(F5.1)
133 23 IF(LONG+AND. NOT.OPT(Y)) PRINT 925
134 835 FORMAT(1X15.5AS TIMES)
135 GO TO 116
136 25 KSHOT(NPTS)=1N00
137 NPTS=NPTS+1
138 DO 29 NAIN+1,NBAD
139 NAIN=(KAIN+O306+END+30) KNCHT(NHAI), (GOOD(NBAD+M),M=1+NCHAN)
140 836 FORMAT(15.5F5.4)
141 28 CONTINUE
142 GO TO 117
143 30 LSHOT(NBAD)=1N000
144 NBAD=NBAD+1
145 IF(MONIT+EQ.0.) GO TO 40
146 C C WE WERE TOLD THE MONITOR CHANNEL #
147 C FIGURE IT OUT (PLAXS IN THE WAVELENGTH FIELD)
148 C 901 FORMAT(' I2 MONITOR SPECIFIED USING CHAN. 1')
149 MONIT+1
150 901 CONTINUE
151 35 CONTINUE
152 C C THERE'S STILL NO MONITOR CHANNEL SPECIFIED...
153 C USE CHANNEL 1
154 C
155 C PRINT 901
156 901 CONTINUE
157 C WE WEREN'T TOLD WHICH TIME TO START WITH...
158 C FIND AVERAGE TIME FOR PFAK OF MONITOR SIGNAL
159 AMONG FIRST 12 RECORDS
160 DO 47 L=1,12
161 CALL TRCAD(HSHT+KEOF)
162 IF(KEOF+EQ.0.) GO TO 118
163 40 IF(KTIME+NE.+0.) GO TO 50
164 47 CONTINUE
165 40 CONTINUE
166 50 MAX+ISIG(MOJIT+1)
167 I=1
168 IF(SIG(MOJIT+K)+LE.+MAX) GO TO 45
169 K=K+2
170
****** READ *****

171 MAX=ISIG(NAWD+1)
172 45 CONTINUE
173 47 KTILE=KITk+1
174 KT14=MIN(57,KT14E/12)
175 CALL READ
176 IF(WIT!L.1)) STOP
177 50 INREC=0
178 MSHOT=0
179 IF(LONG)PRINT 868
180 858 FORMAT(IX/* RECORD SHOT # FIXED DATA*/)
181 DO 82 L=1,NREC
182 82 READ A RECORD
183 83 CALL TREAD(NSHOT,KEOF)
184 IF(KEOF,NE.0)GO TO 85
185 MSHOT=MSHOT+1
186 IF(LONG)PRINT 840+NSHot,ISHot+NUM
187 840 FORMAT(IX/*,19,IX*4,S12,I2,2X,6F2)
188 INREC=INREC+1
189 C
190 END THE WAVELENGTH INFO FOR THIS SHOT NUMBER
191 192 IF(NSHOT.LT.KSHOT(JPTS))JPTS=1
193 IST=JPTS-JPTS+1
194 DO 62 I=IST,ISTOP
195 IF(NSHOT.LT.KSHOT(JPTS+1))GO TO 63
196 62 JPTS=JPTS+1
197 63 CONTINUE
198 DO 82 L=1,NCHAN
199 C
200 LOAD DATA FROM ONE CHANNEL INTO A RECORD
201 202 DISCARD DATA IF DESIRED
203 IF(NCHM,NE.99999.99999)GO TO 82
204 C
205 PICK UP SCALE # FROM RECORD HEADER
206 207 IF(JRE(JPTS))N=NUM(M-1)
208 IF(50+QHT.0)NHT,N,5,1)GO TO 65
209 IF(.NOT.QUET)PRINT 992,INREC,NSHOT,NHT+5
210 NERT=ERROR+1
211 902 FORMAT(* TAPE RECORD,*,SHOT,*,ISHT,*,CHANNEL,*,12,
212 = SCALE # OUT# NHT,*,ISHT,
213 = USING .005 V/DIV)
214 IS=1
215 65 K=KT14
216 C
217 SUBSTITUTE CORRECT AMPLIFICATION IF NEEDED
218 219 AMPLFY=SCALE(IS)
220 66 IF(LSHOT(JBAD),EQ.100000)GO TO 68
221 IF(NSHOT-LSHOT(JBAD))BAD=1
222 IF(LSHOT-LSHOT(JBAD+1))GO TO 67
223 BAD=BAD+1
224 67 IF(JBAD,NE.0)GO TO 71
225 C

ORIGINAL PAGE IS OF POOR QUALITY
****** PRINT ******

220 C PICK UP SAMPLE INTERVAL FROM RECORD HEADER
224 I=I+1 (I)
226 IF(I GT 3 AND I LE 9) GO TO 70
229 NERR=ERR+1
232 IF(I=0)PRINT '03 RECORD SHOT IS', IT=I,
233 903 FORMAT(' TAPE RECORD#4, SHOT# IS,
234 '***SAMPLE INTERVAL # OUT OF RANGE!# IS/
235 'USING .1 MICROSEC')
236 IT=2
237 70 SAMPLE=SCALE(I)
238 C GIVE ONE WARNING IF INTERVAL ISN'T .1 US
239 IF(ISAMPLE.EQ.1 OR WARNED)GO TO 72
241 NERR=ERR+1
242 WARNING=TRUE
243 PRINT 943,IREC,HSHOT,SHOT, SAMPLE
244 943 FORMAT(' TAPE RECORD#4, SHOT# IS,'***SAMPLE INTERVAL .1US',
245 'USING .1 MICROSEC')

246 C TRANSFER DATA POINTS
247 72 TIMESK=SAMPLE
249 GO 73 IF=7...RECORD.2
250 RECORD(XX)=TIME
251 C WE MAKE A CORRECTION OF A FACTOR OF 10 BECAUSE
253 C THERE ARE Too EXTRA AMPLIFIERS IN THE DATA SYSTEM
254 RECORD(XX)=1*ISIG(M)*AMPLFY
255 XX=XX+1
257 75 TIME=TIME+SAMPLE

258 C SET OUTPUT RECORD HEADER
259 ECOUNT(lb0,IREC,HSHOT)JPTS,4*,HSHOT
260 350 FORMAT('b*13)
261 RECORD(3)=AMPLFY
262 IREC(4)=HSHOT
263 WRITE(IFILE,IREC)RECORD
264 82 CONTINUE
265 GO TO 72
267 C END OF FILE...QUITTING TIME
268 85 PRINT 860,HSHOT,IREC
269 860 FORMAT('SHOTS PROCESSED/1X,16** RECORDS WRITTEN')
270 IF(1.GT.0)PRINT 965,LEN
271 965 FORMAT('1X,16** ENDS OR <AMOUNT>)
272 GO TO 199

273 C COMPLAIN
274 106 PRINT 908
276 908 FORMAT(' HEADER CARDS ARE MISSING')
277 GO TO 199
278 108 PRINT 908,HCHAIN,HCHAIN
279 908 FORMAT(' NUMBER OF CHANNELS# IS OUT OF RANGE 1 TO**12)
280 GO TO 199
281 110 PRINT 910,SHOT
282 910 FORMAT(' SAMPLE INTERVAL OF# IS BAD/'
283 'USING TAPE RECORD HEADER')
284 GO TO 12
```plaintext
***** REV REY *****

285  112 PRINT 912,MONIT
286  912 FORMAT('GIVEN MONITOR CHANNEL #**15**, IS RAQ')
287   MONIT=0
288  GO TO 15
289  114 PRINT 914,ACTIVE
290  914 FORMAT('GIVEN STARTING CHANNEL #**15**, IS BAD')
291   KTI=L=0
292  GO TO 15
293  116 PRINT 916,KMPTS
294  916 FORMAT(' THERE ARE MORE THAN**13**, WAVELENGTH CARDS')
295  GO TO 199
296  117 PRINT 917,NWAD
297  917 FORMAT(' THERE ARE MORE THAN**13**, CORRECTION CARDS')
298  GO TO 199
299  118 PRINT 918
300  918 PRINT('FEWER THAN 12 SIGNALS ARE PRESENT')
301  GO TO 194
302  124 PRINT 924,MPCD
303  924 FORMAT('MORE THAN**15**, TAPE RECORDS...QUITTING')
304  C
305  C  CLOSE OUTPUT FILE
306  199 WRITE(INFILE,REC)ENDREC
307  STOP
308  END

**WORK.LJCT

ORIGINAL PAGE IS
OF POOR QUALITY
****** REVERT (Sample data) ******

Long printout is wanted.

All data run on 10 Nov 75; pressure = 185; T = 7V; reflector = .8
3 channels were used.

First shot number at these wavelengths

Channel 1 set at 3280.0 Å
Channel 2 set at 4688.0 Å
Discard data for channel 2, shots 84-92.

Channel 3 is for monitor signal.

Shot 76 had wrong amplifier setting recorded

Channel 1 amplification was .005 V/div
Channel 2 amplification was correctly recorded

Some signals were attenuated

Attenuation factor was .151

Signals for 4670 Å through 4696 Å were attenuated
*****  ENTRY (TREAD)  *****

SUB37JW(LNAME=LNAME(TREAD)
1  *  HAVE***
2  *  DATATAPE
3  *  PURPOSE...
4  *  TO READ THE HIGH SPEED DATA ACQUISITION SYSTEM TAPE.
5  *  CALLING SEQUENCE...
6  *  CALL TREAD (BUFFER+EOF)
7  *  BUFFER 333 WORD DATA INPUT BUFFER; INT*SER
8  *  BUFFER(1) IS THE EXPERIMENT COUNT
9  *  BUFFER(2-13) ARE MISC FIXED DATA
10  *  BUFFER(14-333) THE DATA POINTS; DIMENSIONED (5,64)
11  *  EOF END OF FILE; ANYL. SET 'NON-ZERO' IF EOF
12  *  WAS DETECTED WHEN THIS READ WAS ATTEMPTED;
13  *  ZERO OTHERWISE.
14  *  ONE TAPE RECORD IS READ AND UNPACKED INTO THE USER'S BUFFER
15  *  CALL PEN'TIN
16  *  THE DATA TAPE IS REMOVED.
17  *  INPUT...
18  *  TAPE RECORD FORMAT IS:
19  *  6 BYTES (3CD, 2/BYTE) FIXED DATA
20  *  3 BYTES (8CC) EXPERIMENT COUNT
21  *  320 BYTES (BINARY) DATA GROUPED BY TIME
22  s(i)  AAREX.
23  *  MAIN ENTRY POINT
24  *  TREAD= LA A0+END. ARE WE AT THE END OF THE FILE?
25  *  J+Z A0+3, XI.  IF SO RETURN AT 0NCF
26  *  ANOTHER LA+U A0+PNTT. FETCH A BUFFER FULL
27  *  EN 10%.  PICK UP STATUS AND CHECK
28  *  LA A0+STATU+. SHOULD HAVE AN AFC OF 5
29  *  TE A0+STATUS.  
30  *  J EOF+  OKAY SX XI+SAVEX.
31  *  LAH XI+x0+XI.. XI WILL POINT TO THE NEXT WORD IN THE
32  *  LA+W XI+1.. USER'S BUFFER ALTHOUGH THE PROGRAM
33  *  PICK UP EXPT COUNT
34  *  LA A0+INBUF+1. WIPE OUT EXTRANEOUS STUFF
35  *  AND+U A0+017.  LA A2+AI.
36  *  SSL A0+6.
37  *  AND+U A0+017.
38  *  MSI+U A1+10.
39  *  AA A2+AI.
40  *  SSL A0+6.

ORIGINAL PAGE IS
OF POOR QUALITY
68

***** REVERT (THE) *****

57 ANDU A2+817.
58 M2+U A1+100.
59 AA A2+1.
60 SA A2+0.*X1.
61 * PICK UP MISC DATA
62 * DL A2+1HUF.
63 * SIX BYTES OF TWO CHARACTERS/BYTE
64 LR U H2+5.
65 DSC A9+8.
66 LOOP1 LUSC A9+12.
67 MOVE FORWARD 3 NUMS, PUT IN A1(3-0)
68 ANDU A1+017.
69 MOVF LAST DIGIT TO A2(3-0)
70 SA A2+0.*X1.
71 STORE DIGIT
72 LOOP2 DSC A9+8.
73 MOVE BACK 1 DIGIT
74 ANDU A1+017.
75 PUT ONE DIGIT INTO A2(3-0)
76 SA A2+0.*X1.
77 STORE BCD DIGIT
78 LOOP3 JG R2,LOOP1.
79 DECREMENT COUNTER
80 * GET REAL DATA
81 SX X2+5AVEX+1.*
82 X2+1(p, INUF+2) OF WORDS IN INPUT BUFFER
83 LR U R2+34.
84 MOVE 35 PAIRS OF WORDS (315 BYTES)
85 LOOP4 DL A2+0.*X2.
86 PICK UP TWO PACKED WORDS
87 LR U R1+1.
88 NIUF WBE AT A SHIT
89 LOOP5 LUSC A9+8.
90 ANDU A1+0377.
91 TRANSFER ONE BYTE TO A2(7-0)
92 SA A2+0.*X1.
93 JG R1+LOOEP2.
94 SHIFT UNTIL DOUBLE WORD IS FINISHED
95 LOOP6 D2+0.*X3.
96 PICK UP LAST TWO WORDS
97 LOOP7 LR U R1+1.
98 PROCESS ONLY 5 BYTES
99 * END OF FILE OR TAPE ERROR
100 EOF LA+S1 A3+PKTT+3.
101 TEST FIRST FOR EOF
102 TE+U A0+01.*
103 MEANS END OF FILE.
104 J B3.
105 NOT THAT EOF REACHED
106 LA+H2 A3+PKTT+3.
107 THE U A3+74.
109 SLJ PRINT.
110 LENGTH WRONG...PRINT STATUS
111 ER A9019.*
112 AND QUIT.
113 B1 LA+S1 A3+PKTT+3.
114 GET I/O COMPLETION STATUS CODE AGAIN.
115 THE U A0+00.
116 J OKAY.
117 COPIED TAPE, SINCE FRAME CT IS NORMAL
****** REVLR (THEAL) ******

114 TL+U A0+R24. 04 MEANS ABNORMAL FRAG. COUNT.
115 J R22.
116 SLJ PRINT. ARC NOT S, SO WE PRINT STATUS AND
117 J ANOTHER. GET NEXT RECORD.
118 SLJ PRINT. SOME OTHER I/O ERROR...PRINT STATUS
119 ER ABORTS* AND QUIT.
120 * SUBROUTINE FOR PRINTING OUT THE STATUS WORD
121 *
122 PRINT + S-S +
123 LA A0+PKT+3. GET THE STATUS WORD
124 LR+U R2+1.
125 E2 SA A2*R16UF+1. (USEFUL ONLY ON 2ND ITERATION OF LOOP)
126 LA A1+R15.
127 E1 ANL,U A0+R7. MOVE ONE OCTAL DIGIT TO A1(2-0)
128 AA+U A1+R50. CONVERT TO FIELD DATA DIGIT
129 DSC A1+R6. MOVE INTO A2(35-30)
130 SSL A0+R3. MOVE NEXT OCTAL DIGIT TO A0(2-0)
131 JD R1+E1.
132 JD R2+E2.
133 SA A2*R16UF.
134 LA A0+(0104+INBUF+2).
135 EN PRINTS.
136 J *MKRT+1.
137 *
138 * REWIND ENTRY POINT
139 *
140 REIND* L+U A0+R24. REWIND THE TAPE
141 ER IOWS. CHECK FOR BAD STATUS
142 LASL A0+R6+3.
143 J NZ A0.
144 J HE2.
145 SLJ PRINT. STATUS 9AD...PRINT THE STATUS
146 ER ABORTS* AND QUIT.
147 RE2 S2 END. NOTE WE AREN'T AT AN END OF FILE NOW
148 J NZ1+X.
149 *
150 * STORAGE AREA
151 *
152 *(0)+SAYEX RES 2.
153 PKTT 10: INTAPE+D4, 74+INBUF.
154 "I/O STATUS '.
155 INUF RES 74.
156 STATUS +04U0000012.
157 END + 0 - SET NONZERO WHEN EOF FOUND
158 RWD 10: INTAPE+RE3*
159 END

THEAL

ORIGINAL PAGE IS
OF POOR QUALITY

W+ET
*** REVERT (OPT) ***

Z051/31/1#WORKSPACE(1).OPT

1 * NAME...
2 * OPT
3 * PURPOSE...
4 * TO OBTAIN FOR THE USER PROGRAM THE OPTIONS SPECIFIED ON
5 * THE EXECUTING STATEMENT.
6 *
7 * CALLING SEQUENCE...
8 *
9 * LOGICAL SWITCH=TEST.OPT
10 *
11 * SWITCH=OPT('U')
12 * TEST=OPT('T')
13 *
14 * SWITCH WILL HAVE THE VALUE 'TRUE', IF THE 'U' OPTION WAS
15 * SPECIFIED ON THE XGET OR 'FILE PROGRAM CARD, AND 'FALSE'
16 * OTHERWISE TEST WILL SIMILARLY INDICATE THE PRESENCE OF
17 * THE 'T' OPTION.
18 *
19 * LIT.
20 * A6+3.
21 OPT+ TZ HAVE  * GO GET OPTIONS IF WE HAVEN'T ALREADY
22 J   GET  :
23 GO LA A1.30  :
24 SSL A1.30  :
25 A21 U A1.30  :
26 LA A2.30  :
27 LSSL A0.30 A1  :
28 SSL A0.30  :
29 J   2*X11  :  SHIFT CORRECT BIT TO HIGH-ORDER BIT
30 GET SX X11,WORD  :
31 ER OPTS  :
32 LX X11,WORD  :
33 SA A0.30  :
34 SGZ HAVE  :
35 J   GO  :
36 RETURN RCS 1  :
37 HAVE + 1  :
38 wO'M+ RCS 1  :
39 END  :

*END
NAME... PARAM

PURPOSE...
TO CREATE RECORDS WITH STRICTLY DECREASING MONITOR SIGNALS

USAGE...
Q:PARAN OR QXOT:PARAM

OPTIONS:
A [QXOT 0 ALY] AMPLIFY SLOW SIGNALS WHICH WERE
ATTENUATED WITH A NEUTRAL DENSITY FILTER

LLOW:WHIGH) (FREE) SIGNALS WITH WAVELENGTHS IN THE
RANGE (LOW, WHIGH) WILL BE AMPLIFIED BY 1/294

INPUT...
ACCEPTS FILES CREATED BY PROGRAMS 'RECOVER' OR 'REVERT'.

RECORDS 1 & 2:
[72A1/72A1] FILE HEADER

RECORDS 3-n:
WORDS 1-2: (F5.1) WAVELENGTH, SHOT 
WORD 3: (R) SCALE, VOLTS/DIV
WORD 4: (I) SHOT 
WORD 5: (I) # POINTS IN THIS RECORD
WORDS 6-13: (R) TIMES (USEC)
WORDS 14-21: (R) SIGNALS (V)
RECORD N+1:
'QEOF ' IN FIRST WORD

OUTPUT...
FILE ACCEPTABLE TO PROGRAM 'BSORT'

RECORDS 1,2:
[72A1/72A1] FILE HEADER
RECORDS 3-n:
WORDS 1-2: (F5.1) WAVELENGTH, SHOT 
WORD 3: (R) SCALE (V/DIV)
WORD 4: (I) SHOT 
WORDS 5-20: (R) TIMES OF TIME (USEC), SIGNAL (V)
RECORD N+1:
'QEOF ' IN FIRST WORD

SUBPROGRAMS REQUIRED...
BEGIN:OPT

PARAMETER NRCO=1000
INTEGER OUTFIL, OUTREC, TEST:END1
INTEGER HEAD(20), NHIGH, VALLEY, PEAK
LOGICAL OPT
DIMENSION A(8), B(8), FACTOR(8), LOW(B), WHIGH(B)
EQUIVALENC (A(1), HEAD(5)), B(11), HEAD(13))
***** PARAM *****

72

DATA ENO1,INFILE,OUTFILE,INREC,OUTREC
- */EOF, 10, 15, 0, 0/

DIMENSION X(I),Y(I),A(I)

EQUALS=CONT.(X(I),Y(I))

LOGICAL SAME

CALL BEGIN('PARAM 2,11 G')

KATTEN=1

IF(.NOT.OPT('A'))GO TO 5

PRINT UFO

800 FORMAT(' ENTER ATTEN AND WAVELENGTH RANGE')

DO 3 KATTEN=1,8

READ EOS+END=5*FACTOR(KATTEN),LO((KATTEN),WHIGH(KATTEN))

805 FORMAT(I)

#LO((KATTEN))=LO((KATTEN)=-0.5

WHIGH(KATTEN)=WHIGH(KATTEN)+.05

IF(FACTOR(KATTEN)=1.2)PRINT 901

901 FORMAT('')

3 CONTINUE

KATTEN=8

5 #LO((KATTEN))=KATTEN*79999.

WHIGH(KATTEN)=WHIGH(KATTEN)+.05

DEFINE FILE INFILE(HHOD=(U),INREC)

DEFINE FILE OUTFIL(MRC,H2OUTREC)

C TRANSFER FILE HEADER

DO 5 J=1,2

READ(INFILE,'(HEAD(I),I=1,12))

WRITE(OUTFIL,'(HEAD(I),I=1,12))

5 CONTINUE

READ(INFILE,'INREC')(HEAD(I),I=1,4),N,(X(I),Y(I),I=1,N)

QUIT AT END OF FILE

IF(HEAD(I)=EOF,END)GO TO 50

AMPLFY=1.

REWRITE BAD RECORDS A CORRECT AMPLIFICATION

DECODE(330,HEAD)=AVE

FORMAT(FS,1)

DO 12 KK=1,KATTEN

IF(WAVE.LE.LO((KK))GO TO 12

IF(WAVE.LE.WHIGH(KK))GO TO 14

12 CONTINUE

GO TO 15

14 AMPLFY=FACTOR(KK)

15 CONTINUE

TRANSFER RECORD TO OUTPUT AREA

NMIN=NN(NB)

DO 24 J=N2,1

A(N+I)=X(I)

24 B(N+I)=Y(I)/AMPLFY

SORT POINTS ON TIME

IF(N+1)GO TO 40

DO 25 J=N2,1

SAME=TRUE.

25 DO 25 I=J,J

IF(A(I)=GE.A(I-1))GO TO 25

C TRANSFER FILE HEADER

DO 5 J=1,2

READ(INFILE,'(HEAD(I),I=1,12))

WRITE(OUTFIL,'(HEAD(I),I=1,12))

5 CONTINUE

READ(INFILE,'INREC')(HEAD(I),I=1,4),N,(X(I),Y(I),I=1,N)

QUIT AT END OF FILE

IF(HEAD(I)=EOF,END)GO TO 50

AMPLFY=1.

REWRITE BAD RECORDS A CORRECT AMPLIFICATION

DECODE(330,HEAD)=AVE

FORMAT(FS,1)

DO 12 KK=1,KATTEN

IF(WAVE.LE.LO((KK))GO TO 12

IF(WAVE.LE.WHIGH(KK))GO TO 14

12 CONTINUE

GO TO 15

14 AMPLFY=FACTOR(KK)

15 CONTINUE

TRANSFER RECORD TO OUTPUT AREA

NMIN=NN(NB)

DO 24 J=N2,1

A(N+I)=X(I)

24 B(N+I)=Y(I)/AMPLFY

SORT POINTS ON TIME

IF(N+1)GO TO 40

DO 25 J=N2,1

SAME=TRUE.

25 DO 25 I=J,J

IF(A(I)=GE.A(I-1))GO TO 25
**** PARAM ****

114 $z(i)$
115 $a(i)=a(i-1)$
116 $a(i-1)=z$
117 $s(i)$
118 $b(i)=b(i-1)$
119 $b(i-1)=s$
120 $sames=false$
121 continue
122 if(same) go to 30
123 continue
124 if this is a monitor signal, ensure it's
125 not monotonically decreasing
126 decode(840, head) test
127 if(test eq.) go to 31
128 if(test eq.) go to 31
129 id=
130 go to 44
131 drop=
132 high=
133 valley=
134 peak=
135 ib=1
136 if(0.gt.) go to 32
137 if(d(i).le.(f-apscia+1-n)) go to 32
138 if this is bigger than previous biggest?
139 if(b(high)-b(ib)+drop) go to 32
140 is this drop bigger than previous biggest?
141 peak=high
142 valley=ib
143 note this is biggest drop
144 if(ib.ge.peak) go to 36
145 peak=high
146 valley=ib
147 if this is biggest drop...get rid
148 of points before peak
149 if(ib.ge.peak) go to 42
150 if(ib.ge.peak) go to 42
151 $a(i)=a(peak)$
152 $b(ib)=b(peak)$
153 go to 48
154 go to 48
155 go to 48
****** PARA1 ******

1/1 C
1/2 C GET RID OF POINTS AFTER VALLEY
173 42 ID=VALLEY
174 43 IF(I(I)) GT .001 G0 TO 45
175 $A(I(I))=A(VALLEY)$
176 $B(I(I))=B(VALLEY)$
177 178 GO TO 44
179 C
180 C WRITE A RECORD
181 45 WRITE(OUTFIL=OUTREC)HEAO
182 46 GO TO 10
183 C
184 C CLOSE THE FILE AND EXIT
185 90 WRITE(OUTFIL=OUTREC)ID1
186 91 I=INREC-4
187 92 PRINT 899,1
188 890 FORMAT(IS,1 CURVES PROCESSED)
189 190 STOP
190 END
TO SORT THE RECORDS, FIRST BY WAVELENGTH, THEN BY SHOT #: 

BEGIN:START; SADD; SORO; HADD; HDROP; ADDTO; FINDTO; EFLUSH; EPOP

METHOD: 
ON A FORWARD PASS, EACH RECORD IS READ. IF IT RANKS HIGH
ENOUGH (HIGHER THAN LEAST ONE CURRENTLY SAVED), IF THE
BUFFERS ARE FULL, IT IS SAVED AND, IF THE BUFFERS ARE FULL,
The least one currently saved is written in its place. When
the end of the unsorted portion of the file is reached, all
records being held are exchanged with stored records. The
process is repeated, in alternating directions, until the
entire file is sorted.

INCLUDE STORES; LIST
LOGICAL FOUND
DATA ELSE,EOF */
DATA HF/E(15)/
CALL I BEGIN('SORT2, 01 G')
DEFINE FILE 'FILE(100+20)+UNIT(1)
CALL START
NEXT=2
FOUND=.FALSE.
LAST=0
INCR=1
NPASS=0
NWRITE=0
NREAD=0
SURE=.TRUE.
BEGIN NEW SWEEP
CHANGE=.FALSE.
NPASS=NPASS+1
CALCULATE &X, PFCORE NUMBER
12 IREC=IREC+1
48 IF(IREC+EO.LAST)GO TO 40
49 IF((HASE@.LE.0).AND.(NOT.SURE))GO TO 30
50 IF(HASE@.EQ.15+14)
14 IF(HASE@.EQ. FROM(HASE))GO TO 24
52 READ NEW RECORD
53 CONTINUE
READ FILE 'FILE(I.BUFFER).I=1, LOW
54 NREAD=NREAD+1
55 IF(FOUNU)GO TO 28
STOP STEP IF THIS IS END OF FILE

IF(H(1, BUFFER), NE, ELSE) GOTO 20

FILL(2, TRUE).
LAST=IREC
IREC=IREC-3
GOTO 40

AND THIS RECORD TO SORT STACK

CONTINUE

FROM(BUFFER), IREC
CALL ADD(BUFFER)
BUFF=DEMAND($89)
GOTO 12

WE ARE HOLDING A RECORD WE WANT TO WRITE HERE...

DO 50 THEN ADD IT TO THE SORT STACK

CONTINUE

WRITE(IFILE), IREC(R(HBASE), I=I,LGH)
WRITE=WRITE+1
CALL EPUSH($89)
GOTO 12

THERE'S NOT ENOUGH ROOM TO DO ANY SORTING DURING

CONTINUE

IF(HBASE, LE, 0) GOTO 32
IREC=POF(HBASE)
WRITE=WRITE+1
CALL EPUSH($89)
GOTO 30

32 IREC=LAST

CONTINUE

LAST=EXT
NEXT=IREC+INCR*KNOWN
IF(I, NOT, CHANGE), AND, ((I, NOT, LE, 0)) GOTO 88
KNOWN=0

RECORD DESTINATIONS OF RECORDS TO BE HELD

CONTINUE

I=HBASE
NT0=0
IF(I55, 55, 52)
CONTINUE
CALL ADDTO(I)
I=UP(I)
GOTO 51

SET POINTERS

CONTINUE

J=LAST+INCR*HT0
J=CHMTO
CALL FINDTO(J)
INCR=I, 1, CR
SURE, TRUE.
STOP=STOP
STOP=STOP
SBASE=0

WRITE SORTED RECORDS IN PROPER ORDER

CONTINUE

IF(TOP), 74, 74, 60
IREC=IREC+INCR
***** dsort *****

114 IF(FLRC.GT.FILE(FMNN(TTOP)):GO TO 64
115 61 IF((Iv(JTO)=1)EC)/CE(I):GO TO 60
116 62 JTOP=JTO-1
117 GO TO 61
118 C FILE RECORD THAT WAS HERE IS IN THE SORT
119 C STACK AND CAN BE OVERWRITTEN
120 63 CONTINUE
121 WRITE(FILE,FIEC)(R(I),I;TOP),I=1+LGH)
122 WRITE=WRITE+1
123 64 I=I+1(TOP)
124 CALL EPUTH(TTOP)
125 TTOP=I
126 GO TO 58
127 C FILE RECORD THAT WAS HER MUST BE HELD
128 C AND WRITTEN BACK LATER THIS SWEEP
129 68 CONTINUE
130 READ(FILE,FIEC)(P(I),BUFFER),I=1+LGH)
131 NREAD=NREAD+1
132 WRITE(FILE,FIEC)(R(I),I;TOP),I=1+LGH)
133 WRITE=WRITE+1
134 CALL EADD(BUFFER)
135 ISDOS(I=H(TOP)
136 BUFFER=TOP
137 TTOP=I
138 GO TO 58
139 C ASSIGN DESTINATIONS TO THE RECORDS HELD
140 IS=H(TOP)
141 ITO=0
142 75 IF(I)=2+60,70
143 78 ITO=ITO+1
144 FROM(I)=To(ITO)
145 ISDOS(I=H(TOP)
146 GO TO 75
147 C GO FOR REST OF THIS SWEEP
148 GO FOR REST OF THIS SWEEP
149 CONTINUE
150 IF(Ab(LAST-NEXT).GT.1)GO TO 16
151 C SORTING COMPLETE...REPORT & QUIT
152 PRINT 808,RECORD,FRAME,READ
153 808 FORMAT(IS,RECORDS SORTED/
154 - IS, PASS/
155 - IS, WRITE/
156 - IS, READS/)
157 STOP
158 89 PRINT 905,PASS
159 905 FORMAT(IS, STACKS FOULED UP BY PASS+14)
160 STOP
161 END

Q=EXIT

ORIGINAL PAGE IS OF POOR QUALITY
SUBROUTINE SADD(HERE)

PURPOSE...
TO ADD A RECORD TO THE 'SORTED' STACK

USAGE...
CALLED BY PROGRAM "ISORT"

INCLUDE STORES-LIST
IF(SURE)KNOWN=KNOWN+1
IF(STOP)STOP=10
STOP=HERE
SHERE=HERE
UP(HERE)=0
DOWN(HERE)=0
RETURN

IF(CMPARE(HERE,STOP))20,15,15
ENTER RECORD AT TOP OF STACK
UP(STOP)=HERE
UP(HERE)=STOP
RETURN

CHANGE=.TRUE.
IF(CMPARE(SHERE,SPACE))22,25,25
ENTER RECORD AT BASE OF STACK
DOJN(SHERE)=HERE
DOWN(HERE)=0
SHERE=HERE
RETURN

I=STOP
DOJN=HERE
IF(CMPARE(HERE,1))30,35,35
ENTER RECORD ABOVE RECORD 1
DOJN(I)=HERE
UP(I)=UP(1)
DOWN(I)=HERE
RETURN
END
**STORES**

**PROCEDURE NAME...**
STORES

**PURPOSE...**
TO COMMUNICATE THE RECORD STACK INFORMATION FOR SORTING PROGRAM 'BSORT'.

**USED BY PROGRAMS...**

**BSORT-BEGIN-START-SADD-SDROP-MADD-MDROP-ADDTO-FINUTO-EPUSH-**

**LL** IS THE NUMBER OF RECORDS HELD IN MEMORY,
AND MUST BE AT LEAST 3

**PARAMETER LL=2**
PARAMETER LGH=20

**IPPLICIT INTEGER [A-Z]**

**DEFINE RECORD(LOC)=IF(LJLJ,LOC),LJLJ+LGH**

**INCR=SURE,CHANGE**
**KNOWN=IT0,IT0=BUFFER**

**STOP=HTOP,FTOP,SBASE,HBASE,**

**DOWN(LL)+UP(LL)+FRO=1(LL)+TO(LL)+R(LGH+LL)**

**LOGICAL SURE,CHANGE**

**END**

**BSORT (START)***

**SUBROUTINE START**

**PURPOSE...**
TO INITIALIZE STORAGE FOR PROGRAM 'BSORT'.

**INCLUDE STORES-LIST**

**BUFF=1**
**ETOP=2**
**DO 1 I=3,LL**

**DOWN(1)=1**
**DOWN(LL)=0**

**STOP=0**
**SBASE=0**
**HTOP=0**
**HBASE=0**
**INCR=1**

**RETURN**
**END**

---

**ORIGINAL PAGE IS OF POOR QUALITY**
*** JSort (SOMOP) ***

0573JM, OMKSPACE=11, 'SORP
1    INTEGER FUNCTION SORP(S)
2
3    PURPOSE...
4    TO DROP A RECORD FROM THE 'SORTED' STACK
5
6    USAGE...
7    CALLED BY PROGRAM 'CSORP'
8
9    INCLUDE STORES.LIST
10    IF(SUASE)0=9S+5
11      SOMOP=SBASE
12      SBASE=UP(SUASE)
13      IF(SBASE)=10,16,19
14      10 STOP
15      RETURN
16      15 DOWN(SUASE)=0
17      RETURN
18      90 PRINT 901
19      901 FORMAT(' SORT STACK OVERWRODE')
20      RETURN 1
21      END
SUB37JHLWORKSPACE$(1), IAND
1 SUBROUTINE IAND(HERE)
2 C PURPOSE...
3 C TO ADD A RECORD TO THE 'HOLD' STACK
4 C
5 C USAGE...
6 C CALLED BY PROGRAM 'D50RT'
7 C
8 C INCLUDE STORES+LIST
9 C IF(HTOP)<5
10 S HTOP=WHERE
11 H BASE=WHERE
12 UP(HERE)=150
13 DOWN(HERE)=0
14 RETURN
15 10 IF(CMPARE(HERE+HBASE))15*20
16 C ENTER TO BOTTOM OF STACK
17 C 15 DOWN(HBASE)=HERE
18 19 UP(HERE)=HBASE
20 20 DOWN(HERE)=0
21 22 H BASE=HERE
22 23 RETURN
23 24 C ENTER TO TOP
24 25 UP(HTOP)=HERE
26 27 DOWN(HERE)=HTOP
28 29 HTOP=HERE
30 RETURN
30 35 IF(CMPARE(HERE+HTOP))35*30
35 C ENTER ABOVE ELEVEN 1
35 36 =UP(HERE)
36 37 DOWN(HERE)=HERE
37 38 UP(HERE)=HERE
38 39 RETURN
40 END

ORIGINAL PAGE IS OF POOR QUALITY.
****** BSORT (HMOH) ******

20537JIM*HKSPACE(1).HMOH
1 INCLUDE FUNCTION HMOH(5)
2 C PURPOSE...
3 C TO DROP A RECORD FROM THE HOL Stack
4 C
5 C USAGE...
6 C CALLED BY PROGRAM 'BSORT'
7 C
8 C INCLUDE STORES LIST
9 C IF(HDASE)=90..90,5
10 C HDFHASE=HBASE
11 C IF(HDASE)=10.10.15
12 C HP=O
13 C RETURN;
14 C Down(HDASE)=O
15 C RETURN;
16 C PRINT 902
17 C 902 FORMAT(' HOLD STACK OVERFLOWED')
18 C RETURN 1
19 END

--------

****** BSORT (ADTO) ******

20537JIM*HKSPACE(1).ADTO
1 SUBROUTINE ADTO(I)
2 C PURPOSE...
3 C TO ADD A RECORD TO THE 'TO' STACK
4 C
5 C USAGE...
6 C CALLED BY PROGRAM 'BSORT'
7 C
8 C INCLUDE STORES LIST
9 C STOP IF STACK IS FULL
10 C NTOS=NTO+1
11 C IF(NTOS,ST,LL) GO TO 90
12 C FIND PROPER PLACE TO INSERT RECORD
13 C CALL FINDTOCI)
14 C MOVE REST OF RECORDS & INSERT NEW ONE
15 C J=NTO
16 C J=J-1
17 C IF(J<LE)(J+1) GO TO 10
18 C TO(J+1)=TO(J)
19 C NTOS=NTOS+1
20 C IF(NTOS,ST,LL) GO TO 90
21 C 18 TO(I)=FROM(I)
22 C RETURN;
23 C PRINT 708
24 C 708 FORMAT(' NTOS GT. LL')
25 C STOP
26 END

Q*EJCT
**BSORT (FIND)**

SUBROUTINE FIND( ITO )

C PURPOSE...
SET POINTER ITO TO POINT IN 'TO' STACK WHERE
A GIVEN NEW RECORD SHOULD BE INSERTED

C USAGE...
CALLED BY PROGRAM BSORT

INCLUDE STORESLIST

END

**BSORT (EPUSH)**

SUBROUTINE EPUSH(LOC)

C PURPOSE...
TO STORE A LOCATION IN THE 'EMPTY' STACK

C USAGE...
CALLED BY PROGRAM BSORT

INCLUDE STORESLIST

END

**BSORT (EPOP)**

INTEGER FUNCTION EPOP(*)

C PURPOSE...
TO GET A LOCATION FROM THE 'EMPTY' STACK

C USAGE...
CALLED BY PROGRAM BSORT

INCLUDE STORESLIST

END
**PROFILE**

**NAME**... PROFILE

**PURPOSE**... TO UNFOLD THE DATA INTO INTENSITY VS WAVELENGTH CURVES

**USAGE**...

Q. PROFILE OR EXIT .PROFILE

**OPTIONS:**
- A PRINT AND WRITE TO OUTPUT FILE POINTS FOR ALL
- B MONITOR INTENSITIES (OTHERWISE: IF < 50% OF THE POINTS ARE ACCEPTED, THE WHOLE PROFILE IS DISCARDED)
- C DISCARD POINTS WITH TIMES FOR THIS MONITOR INTENSITY FURTHER THAN 1.6 SIGMA (DEFAULT 1.73) FROM THE MEAN
- D THROUGH DELETING ABOUT 111 (DEFAULT 86)
- E FILE 10 DATA POINTS OVERPOTS (C' OPTION)
- F PROVIDE FULL LISTING (OTHERWISE, ONLY A SUMMARY)
- G REPORT RESULTS FOR ALL WAVELENGTHS (EVEN IF MOST POINTS ARE DISCARDED)
- H SKIP SOME PROFILES
- I GENERATE FILES FOR PROGRAM 'THEORY'

**SUBPROGRAMS REQUIRED...**

BEGIN,OPT,TIM,INTENS,LOOKUP,YESNO

**PARAMETER LINEXP=36**

**PARAMETER LMAXP=30**

**PARAMETER LMAXP=32**

**PARAMETER LSH=(8)**

**PARAMETER CSIZE=360**

**PARAMETER CSIZE2=CSIZE+2**

**DIMENSION MU,LH,LHEXP,LHSH,LENGTH(LINEXP)**

**DIMENSION BLOCK(59),EVOLTE(2)**

**EQUIVALENCE (INTREF,LOOK(1)) , (TAV,LOOK(2)), (J,LOOK(3))**

**INTEGER TEMP(20),GRP**

**DIMENSION HEADER(24),SIG(LINEXP),ERROR(LINEXP),LREL(20)**

**EQUIVALENC E (TEMP (4),SHOT) , (TEMP (5),AREF(I)) , (TEMP (13),BREF(I))**

**EQUIVALENCE (LABEL(4),HSHOT) , (LABEL(5),ALIN(I)) , (LABEL(13),ALIN(I))**

**DIMENSION AREF(I),BREF(I),ALIN(I),ALIN(I),LOCATE(CSIZE)**

**INTEGER SKIP(10),PRINT,CLOSE ALL,THEORY,PR5KIP,EVRY**

**LOGICAL YESNO,REPORT**

**REAL INTENS,TAV(LINEXP),LAMDA,LENGTH,INTREF**

**REAL BEGIN,INTER**

**EXTERNAL INTER**

**INTEGER POOR,EALY,FOUND,PCE**

**INTEGER GROUP(8),BEGIN(8),END(8),GREG+FILE,PREC/1,GP,TY,OUT**

**INTEGER RSHOT,REFDIR,REFI,CMEO,CFILE,E1,POIN'TS,BAD**

**INTEGER SHOT(LINEXP,10),TAG(LINEXP,10),INTAG(10),LINTAG(LINEXP)**

**INTEGER TFILE,TRC,TPAT**

**DATA (BLOCK(I)),I=1421/180*/
**PROFILE**

57  DATA INFIL1, DEL1, LDA, NONQOF, RFI1, CFIL1, FILL, TFM
58  / 15, 1, *GUF 1, U.B, C>, 0, 10, 21, 20,5/  
59  DATA LIT(11); ALTER-SPRD-EVNIOT
60  / 132, 85, 3, *, 1, /
61  CALL LEND('PROFIL1 2.41 21)
62  DEFINE FILE INFIL1: IFI1, 25, U, INREC)
63  DEFINE FILE CFIL1(I-SSIZ4), D1, U, INREC)
64  C  FIND OUT WHETHER TO PRINT PROFILE OUT
65  ALL =OPT('TA')
66  C  CLOSE =OPT('C')
67  EVERY =OPT('E')
68  PRINT =OPT('P')
69  REPORT =OPT('R')
70  PRESKIP =OPT('S')
71  THEORY =OPT('T')
72  IFICLOSESPREAD=2.56
73  IF (.NOT.EVERY) GO TO 65
74  EWNOT(1)= 'IIC'
75  EWNOT(2)= tUINDED 
76  IF (.U&T.THEORY) TFILEO
77  IBEG(1)= 0.0
78  C  SAVE FILE HEADER
79  L=0
80  X=0
81  C  READ(INFIL1,HEADER(1),1=1,12)
82  C  READ(INFIL2,HEADER(2),1=11,24)
83  C  FIND BEGINNING AND END OF EACH GROUP
84  10 READ(INFIL1,THREC),LABEL
85  IF(LABEL(1),0.E,11,GO TO 25
86  DECODE(800,LABE1),1RP
87  860 FORMAT(5)
88  DECODE(803,LABE1),R
89  863 FORMAT(1)
90  GP=GP+100
91  IF(1GHP.D.E,1.*100 To 12
92  INREC(1)= MAX(NCSTART,L(1))
93  END(1)
94  LOCATE(1)= NCNEW
95  12 =0
96  15 =1
97  IF(IAT,GO TO 20
98  IF (GROUP(1,M.GP),0=GP,ST,103, GROUP(1,1)) GO TO 19
99  GO TO 19
100  C  FOUND BEGINNING OF NEW GROUP
101  20 IFIL1,CE,AGO TO 197
102  L+1
103  GROUP(L,1) GP=100
104  PRECG(1)=INREC-1
105  PRINT GP,5GROUP(L),PSEGIN(I),
106  805 FORMAT(1) FOUND GROUP: '197' AT RECORD',141
107  IF (LE,END(L)=INREC-2
108  GO TO 10
109  25 IFIL1,GEREND(L)=INREC-2
110  C  NOTE BEGINNING & END OF REFERENCE SIGNAL GROUP
111  INREC=1
112  K=0
113  GO 30 K=1,L
***** PHIOLE *****

114 30 IF(GI(KK) .LT. GI(U)) GO TO 32
115 GO TO 191
116 32 REF=BEGIN(KK)
117 REF=END(KK)
118 KK=0
119 KLINE=I
120 J流水
121 IF(II .GT. K) PRINT 906
122 806 FORMAT('FILES INTENSITY POINTS'/
123 = (VOLS) FOUND BAD')
124 C PRODUCE NEW FILE FOR EACH LINE PRESENT
125 C 00 100 KK=KLINE
126 C INITIALIZE THE FILE
127 35 KK=KK+1
128 IF(KK .GT. KLINE) GO TO 190
129 IF(GROUP(KK) .EQ. 0) GO TO 35
130 PFILE=CFILE+K
131 CAEC=I
132 JS=BEGIN(KK)
133 JS=END(KK)
134 IF(JJ .LT. JA+1) GO TO 190
135 DO 30 J=JA,JO
136 REAC(FILE*,J),LABEL
137 30 WRITE(CFILE*,CFILE,LABEL
138 CEND=KCC-1
139 CFILE=FILE(14,3*LI EXPI,UPREC)
140 WRITE(CFILE*,HEADER
141 INT=t=I
142 TRY=1
143 N=0
144 LINES=100
145 IF(N .GT. THEORY) GO TO 40
146 DEFINE FILE TFILE(13,55+(2*LISH)+LINEXP+TREC)
147 WRITE(TFILE*,HEADER
148 C START NEXT MONITOR SIGNAL LEVEL
149 40 INT=AL+1 INT=I
150 TRY=TRY+1
151 IF(TRY .EQ. 20) GO TO 97
152 IF(II .GT. K) GO TO 41
153 PRINT EFILE,TFILE*INT=I
154 IF(YEAR .EQ. WHITE) GO TO 97
155 N =0
156 GO TO 40
157 41 AVERAGE=0
158 CNAME=I
159 J=1
160 LENGTH(I)=2
161 POINTS=U
162 NPOP=0
163 FOUND=0
164 POOR=0
165 BAD=0
166 OUT=0
167 EEARLY=0
168 LATE=0
169 N=0

ORIGINAL PAGE IS
FOR POOR QUALITY.
****** PROFILE ******

171 C FIND MEAN & STANDARD DEVIATION OF TIMES FOR THIS
172 C MONITOR INTENSITY.
173 C IF(INT.GT.1) GO TO 44
174 C
175 C WE MUST READ THE FILE THE FIRST TIME THROUGH
176 C
177 DO 44 L=1,41,1
178 READ(INFILE,L)TF1
179 NT=1
180 T=T+A
181 TS=TS+TA
182 42 CONTINUE
183 GO TO 50
184
185 C RECORD TIMES FOR ALL MONITOR SIGNALS NOT USED
186 C FOR THIS PROFILE
187 DO 44 L=1,41,1
188 CALL LOOKUP(Locate(L+1-REF1)+1,LIST+1)
189 READ(INFILE,L)TEP
190 T=TEP (INTREF,AREF,REF1,TF1,TF45)
191 T=T+FA
192 NT=NT+1
193 TS=TS+TA
194 45 CONTINUE
195 GO TO 50
196 CALL EMPTY(LIST)
197 TAVE=T/FLOAT(N)
198 TSIGN=FLOAT(TS-TAVE)*FLOAT(NT-1)
199 TSIGN=FLOAT(TS-TAVE)*FLOAT(NT-1)*SPREAD
200 T=0
201 TS=0
202 NT=0
203 INREC=REF1
204 NSHO=2
205 C GET ANOTHER CURVE UNLESS WE'RE AT THE END OF THE FILE
206 IF(INC+2,LE,C.EQ.0) GO TO 50
207 C IF WE HAVE DATA FOR THIS WAVELENGTH, FIND AVERAGES
208 IF(IN,G.EQ.0) GO TO 70
209 C IF WE HAVE DATA FOR THIS TIME GO RECORD IT
210 IF(J.GT.1) GO TO 81
211 C GO TO NEXT TIME
212 GO TO 90
213 C GET NEW CURVE
214 READ(CFILE,C(MIN1,CPE.CLABEL
215 DEC0E(18+1,1+1),LAEL,LAEL
216 812 FORMAT(5I4)
217 IF(AJ5(LAMBDA-LH=-H11) .LT. .021) GO TO 58
218 IF(I.GT.0) GO TO 70
219 56 LENGTH(J)=LAMBDA
220 N0=0
221 NF=0
222 C GET REFERENCE CURVE FOR THIS SHOT
223 IF(INC+2.LE.AFFEND) GO TO 50
224 NF=M(NF+1,10)
225 SHOT=SHO
226 IF(J.GE.1) GO TO 81
227 INREF1

ORIGINAL PAGE IS OF POOR QUALITY
GO TO 60
59 IF LOCATE(INREC*1=REF1),500,SHOT1 GO TO 60
I=INREC
60 DO 61 I=REF1,REIF C
61 IF LOCATE(INREC*1=REF1),500,SHOT1 GO TO 63
C NO MONITOR SIGNAL FOUND FOR THIS SHOT IN FILER!
C INREC=I
C NO=NO+1
C TAG(J,NF)=N'
GO TO 52
63 READ(INFILE*INREC)ENP
C RECORD TIME AT EXT INTENSITY
TA=TI+(INTREF*AREF*60+66+*193)
NT=NT+1
NT=NT+TA
TS=TS+TA*TA
C IF TIME FOR THIS MONITOR INTENSITY IS MORE THAN
C 1.73 (OR 1.6 UNDER *C OPTION) SIGMA FROM THE MEAN,
C THE MONITOR SIGNAL IS BAD AND WE DISCARD THIS POINT.
C THIS SHOULD ASSUMING A GAUSSIAN DISTRIBUTION
C DELETE ABOUT 8% (OR 1%) OF THE POINTS.
64 TA=TI+(INTREF*AREF*60+66+*193)
IF(TA-TAVER..LT.TSIG)GO TO 65
POOR=POOR+1
C FOUND ONE MORE CURVE FOR THIS LEVEL...RECORD
C 65 N=N+1
IF(N-GT-L,.SH)GO TO 16
C IF(N-GT-L,.SH)GO TO 16
C INT(I)=INT(1,SHRT+BLIN,*67+506)
SKIP(I)=.FALSE.
NTAGN=N'
GO TO 52
C INTENSITY IS OUT OF RANGE OF MONITOR VALUES
66 OUT=OUT+1
C TAG(J,NF)=T0'
GO TO 69
50 EARLY=EARLY+1
67 EARLY=EARLY+1
C IF(CONT.GO.TT.10)GO TO 97
58 LATE=LATE+1
C IF(CONT.GO.TT.10)GO TO 97
69 N=N-1
GO TO 52
C FOUND ALL DATA FOR ONE WAVELENGTH...
50 CALCULATE AVERAGE INTENSITY
70 RETURN=.FALSE.
71 N=N
SUM=0
SUM2=0.0
DO 72 1=1,N
72 IF(SKIP(I))GO TO 72
73 N=N+1
SUM=SUM+INT(I)
***** FILE *****, 89

285  SUMw=SUM(SUM(I(I=1 IF(I))
286  I.IEA(I,J)=INT(I)
287  CONTINUE
288  IF(N=175,75,72)
289  NDJ=SUM(NJ)
290  IF(NJ=175,75,73)
291  SIG(J)=SUM(SUM(INTAV(J)/NJ-1)
292  IF(SIG(J)<1.E-6.D0,.P.EQ.O))GO TO 76
293  DISCARD POINTS ONLY ONCE
294  REMOVAL OF ALL POINTS FURTHER AWAY THAN 1.8 SIGMA
295  THIS SHOULD DELETE ABOUT 6% OF THE POINTS.
296  DO 74 IT=1,N
297  IF(SKIP(I))GO TO 74
298  IF(I<INTAV(J)*2.*LT.SIG(J)+3.24)GO TO 74
299  BND=N+1
300  I=INTAG(I)
301  T=INTAV(J)="U"*
302  IF(T<AVR7)GO TO 74
303  RETURN=.TRUE.
304  IF(SEMAG(I))=TRUE.
305  C 74 CONTINUE
306  C  IF(REPORT)J=J+1
307  C  PRINT 870
308  C  FORIAT(0,1,E,N) MORE THAN 14Η, WAVELENGTHS, REST DISCARDED *****
309  C  DO18 OTHER RECORDING OR PRINTING IF MORE THAN 40% OF THE POINTS WERE THROWN OUT
310  C  GO TO 74
311  C  75 INTAV(J)=SUM
312  C  SIG(J)=0.
313  C  76 SIG(J)=3RT(SIG(J))
314  C  IF(SIG(J)<1.E-6.D0,.P.EQ.O))GO TO 74
315  C  ERROR(J)=10.^5.SIG(J)/INTAV(J)
316  C  AVERAGE=AVR7+ERROR(J)
317  C  LINTAG(J)=AVR7
318  C  POINTS=POINTS+1
319  C  J=J+1
320  C  GO TO 80
321  C  79 IF(REPORT)J=J+1
322  C  FOUND=FOUND
323  C  IF(CREC.GT.CENT)60 TO 81
324  C  IF(JLE.LINXL)60 TO 95
325  C  J=J+1
326  C  PRINT 950
327  C  980 FORMAT(*.0000 MORE THAN 14 Η, WAVELENGTHS, REST DISCARDED *****)
328  C  DONT OTHER RECORDING OR PRINTING IF MORE THAN 40% OF THE POINTS WERE THROWN OUT
329  C  GO TO 74
330  C  81 FOUND=FOUND+1.POOR+OUT+FAPL+LATE
331  C  IF(FINDQ.LE.0)60 TO 195
332  C  PCENT=(100*N(POOR+OUT+FAPL+LATE+BAD))/FOUND
333  C  J=J-1
334  C  IF(ALL)GO TO 82
335  C  IF(PCENT.GT.40)GO TO 92
336  C  IF WAVELENGTH IS IN UV DIVIDE BY TWO
337  C  TO COMPENSATE FOR INCORRECT MCPherson SCALE
338  C  82 IF(LENGTH(I),GT.,3300.)60 TO 86
339  C  DO 84 IT=1,J
340  C  84 LENGTH(I)=5*LENGTH(I)
341  C  86 IF(PRINT)GO TO 87

***PROFILE***

```fortran
90 PRINT B13,PFLE,TFLE,INTREF,FOUND,PCTN
91 FORMAT(1X,12,13,5A3,F9.3,I9,15,1H)
GO TO 91
C
97 LINES=LINES+J+17
IF(HEAD.LT.0)GO TO 88
IF(LINES.LT.57)GO TO 99
88 PRINT B14,HEADER
814 FORMAT(1H1,12A6/IH.
815 FORMAT(HI.12A6/IH.
LINES=J+19
99 PRINT B15,TAVEP,TSIG4A,INTREF,PFLE,FOUND,PCTN
= POOR+EVNOTE.OUT+EARLY+LATE+BAD+EVNOTE.POINTS
815 FORMAT(1X,TIME='**F6.3,+**F5.3,**HSEC  MONITOR =,**
96+V FILES*'I3+I5+I1W)
90 PRINT 816
365 FORMAT(' AVERAGE LENGTH   INTENSITY   ERROR**T30**POINTS FOUND**/
366 - FORMATION (ANGSTROMS) (VOLTS)**)
367 DO 90 I=1,J
368 II=I+TAG(I)
369 PRINT B18,LNGTH(I)+I+TAG(I),SIG(I),ERROR(I),
370 - (SHOT(I+1)+TAG(I,I)+II+I+ITT)
371 B18 FORMAT(F10.2,F9.5,+**F7.5**F6.0,T35,1H%)
372 - 2X(101+F4+I)1)
373 AVERAGE=AVERR(I)
374 PRINT 821,AVERR
376 PRINT 821,TITI**AVERAGE SIGMA**F6.0+T35,1H%)
777 C
778 WRITE FICATION TO FILFS
779 IF(WAVE+29)LENGTH=II+J=20.
WRITE(0FILE+PRECI)**TRE**LENGTH+I+TAU**SIG
780 IF(HEAD)WRITE(0FILE+TAG)=LOCK, IN LENGTH, INEXP
GO TO 96
C
92 NPROF=NPROF+1
93 IF(10,19)GO TO 96
C
92 REPORT ONE PROFILE DISCARPE)
95 IF(10,19)GO TO 96
C
GO TO NEXT PAGE IF THIS PAGE HAS A PROFILE ALREADY
94 PRINT B29+INTREF,PCTN,HOMON,POOR+OUT+EARLY+LATE+BAD
825 FORMAT(' MONITOR =**F5.3,**% DISCARDFD**/)
825 - **I**1**, **I**4**, **P**4**, **D**4**, **E**4**, **L**4**, **B**4**)
91 - IHEAD=1
92 GO TO 96
C
C
C
REPORT ERRORS OCCURING WITHIN MAJOR LOOP
C
180 PRINT 901+GROUP(II)+J+I+CFILE+CIZE
901 FORMAT(' GROUP'=**I5*'**USES RECORDS**I4**THROUGH*I4**

-
**FILE**

```
     399      '...TOO MANY FILES!
     400      ' WHICH HOLDS*** RECORDS*
     401      GO TO 97
     402      192 PRINT 902,INTREF
     403      902 FORMAT(' MONITOR 2=#F5.3,1; TOO FEW VALID MONITOR SIGNALS')
     404      GO TO 40
     405      193 PRINT 903
     406      903 FORMAT(' INVALID DATA IN RECORD#13,** GROUP 1,2,6,** SCALE=F6.3,
     407                     -X, SHOT/I4/
     408                     \X,8F8.5/I,8F8.5)
     409      194 PRINTF='FOUND*MONITOR=OUT*EARLY*LATE
     410      195 PRINT 904,J,INTAV(J)+1,J=1..20
     411      904 FORMAT(' ERROR ON POINT#13,**F6.2,**AV INTENSITY=F6.5/
     412                     F7) FOUND#13,** POINTS USING THE FOLLOWING#13,1**)
     413      905 FORMAT(1X/ PREVIOUS POINTS...)
     414      PRINT 915,TAVERTSIG(J),TREFPFILE+F0N(I),MON,
     415                     60 TO 90
     416      906 FORMAT(1X/ PREVIOUS POINTS...)
     417      PRINT 916,TAVERTSIG(J),TREFPFILE+F0N(I),MON,
     418                     60 TO 90
     419      FINISH FILL
     420      96 IF(PREC.LT.13 .AND. (PCENT.LT.40 .OR. PREC.LT.4))GO TO 40
     421      97 IF(PREC.LE.14)WRITE(PFILL,PREC1E1)
     422      98 IF(PREC.LE.14)WRITE(PFILL,PREC1E1)
     423      99 IF(PREC.LE.14)WRITE(PFILL,PREC1E1)
     500      100 CONTINUE
     501      STOP
     502      REPORT ERRORS OCCURRING BEFORE MAJOR LOOP
     503      190 PRINT 910
     504      910 FORMAT(' NO CURVES FOUND FOR MAIN SIGNAL')
     505      STOP
     506      191 PRINT 911
     507      911 FORMAT(' NO CURVES FOUND FOR REFERENCE SIGNAL')
     508      STOP
     509      197 PRINT 917,LF,GRUP(I),1=1..13,6P
     510      917 FORMAT(' MORE THAN**13,** GROUPS FOUND')
     511      (81B)
     512      STOP
```

ORIGINAL PAGE IS OF POOR QUALITY
**PROFILE (TIM)**

20573JIMKSPACE(1),TI

FUNCTION TIM(INT,A,B,S)

C PURPOSE...

C TO FIND THE TIME CORRESPONDING TO A GIVEN INTENSITY

C USAGE...

T=TIM(INT,A,B,60+90)

C TIM R=0 CALCULATED TIME

C INT R=I GIVEN INTENSITY

C A R=I ARRAY OF TIMES

C B R=I ARRAY OF CORRESPONDING INTENSITIES

C $90 S=I EXIT USED IF DESIRED INTENSITY IS OUTSIDE THE

C RANGE OF THE INTENSITIES IN ARRAY B

C $90 S=I EXIT USED IF GIVEN DATA IS INVALID

C (I.E., TIMES NOT INCREASING OR INTENSITIES NOT

C DECREASING)

C METHOD...

C LINEAR INTERPOLATION.

C REAL INT

C DIMENSION A(B),B

C IF(A(B).LT.A(I)).OR.(B(I).GT.B(I))RETURN 5

C IF((INT.GT.B(I)).OR.(INT.LT.B(I)))RETURN 4

C DO 10 1=2,A

C IF(INT.GE.B(I))GO TO 12

C 10 CONTINUE

C 12 IF(B(I).GE.B(I-1))GO TO 15

C 11 TIM=A(I)

C 12 RETURN

C 13 TIM=TIM=A(I)-A(I-1))*(B(I)-INT)/(B(I)-B(I-1))

C 14 RETURN

C 15 END

W-EXIT
**PROFILE (INTENS)**

203373 INPUT (INTENS(TIME,A,A+B,5,S))
1 REAL FUNCTION INTENS(TIME,A,B,5,S)
2 C
3 C PURPOSE...
4 C TO FIND THE INTENSITY FOR A GIVEN TIME
5 C
6 C USAGE...
7 C Y = INTENS(TIME,A,B,5,S)
8 C
9 C TIME R I GIVEN TIME
10 C A R I SAMPLE TIMES
11 C B R I SAMPLES (INTENSITIES)
12 C $90 S O ERROR EXIT TAKEN IF GIVEN TIME TOO EARLY
13 C $90 S O ERROR EXIT TAKEN IF GIVEN TIME TOO LATE
14 C
15 C METHOD...
16 C LINEAR INTERPOLATION
17 C
18 C DIMENSION A(B),B(A)
19 C IF(TIME.EQ.A(I)) RETURN 4
20 C IF(TIME.EQ.A(I)) RETURN 5
21 C DO 10 I=2,B
22 C 10 CONTINUE
23 C IF(TIME.EQ.A(I)) GO TO 12
24 C 12 CONTINUE
25 C 15 CONTINUE
26 C RETURN
27 C 28 RETURN
28 C END

**ORIGINAL PAGE IS OF POOR QUALITY**
***** I/OFILE (LOOKUP) *****

SUBROUTINE LOOKUP(NUMBER,LIST,S)

C NAME...
C TABLE LOOKUP
C PURPOSE...
 TO CREATE, AND LATER FIND ENTRIES IN A SORTED TABLE OF
 INTEGERS.
C USAGE...

CALL EMPTY (LIST)  MARK LIST AS EMPTY
LIST I:10 WORK ARRAY (SAVED BETWEEN CALLS)
 LIST(1) SHOULD BE SET TO THE LENGTH OF THE ARRAY.
CALL ENTER (NUMBER,LIST,S) ADD NUMBER TO LIST
NUMBER I:1 I NUMBER TO BE ADDED
$ S:1 THIS RETURN TAKEN IF LIST IS ALREADY FULL
CALL LOOKUP (NUMBER,LIST,S) SEARCH FOR NUMBER IN LIST
NUMBER I:1 I NUMBER TO BE FOUND
1 I:0 RELATIVE LOCATION IN LIST, IF FOUND
$ S:1 THIS RETURN IS TAKEN IF NUMBER IS FOUND
 (OTHERWISE, NORMAL RETURN)

DIMENSION LIST(50)
IF(LIST(2).LT.3)RETURN
DO 20 I=3,LIST(2)
20 IF(LIST(I).EQ.NUMBER)RETURN 3
DO 35 I=3,LIST(2)
35 IF(LIST(I).EQ.NUMBER)RETURN 3
ENTRY ENTER(NUMBER,LIST,S)
LIST(1)+=1
IF(LIST(1).LT.2)LIST(2)=2
LIST(1)=NUMBER
RETURN
ENTRY EMPTY(LIST)
LIST(2)=2
RETURN
END

*END
***** PROFILE (YES, NO) *****

*PURPOSE*
TO OBTAIN A YES OR NO ANSWER TO A QUESTION FOR AN INTERACTIVE PROGRAM.

*CALLING SEQUENCE*

*LOGICAL YESNO*

IF(YESNO('SHALL I SKIP OPTIONAL PART?', 'NO')) GO TO 40
CONTINUE

IF(YESNO('SHALL I REPEAT OPTIONAL PART?', 'NO')) GO TO 20

90 <SPECIAL SECTION FOR END-OF-FILE RETURN>

THE QUESTION MUST END WITH THE STOP CHARACTER Q (WHICH ISN'T PRINTED); ON THE QUESTION WILL BE FOLLOWED BY A "WHILE STOPPING TRASH" AND THE PROGRAM MAY BLOW UP. THE QUESTION WILL BE PRINTED, AND THE TELETYPE WILL WAIT ON THE SAME LINE FOR THE USER TO TYPE HIS ANSWER. THAT ANSWER MAY START IN ANY COLUMN AND CONSIST OF ANY NORMAL AFFIRMATIVE OR NEGATIVE WORD (I.E., ANY ONE I COULD THINK OF WHEN I WROTE IT). THE USER MAY SUPPLY AN EOF RETURN ADDRESS AS THE SECOND ARGUMENT, BUT THIS IS OPTIONAL (THE PROGRAM WILL FIND IT'S WAY BACK EITHER WAY).

CONTENTS OF ALL REGISTERS EXCEPT AO ARE SAVED.

*ERROR CONDITIONS*

IF THE USER'S ANSWER IS A BLANK LINE OR A CHARACTER STRING THE PROGRAM DOESN'T RECOGNIZE (IT CAN BE FOOLED) IT TRIES AGAIN, PRINTING ONLY "WHAT?". IT WILL REPEAT THE ORIGINAL QUESTION ONE TIME IN FOUR.

IF THE RESPONSE IS QEOF, THE PROGRAM USES THE ALTERNATE RETURN ADDRESS, IF SUPPLIED, THIS CAN BE USED TO TERMINATE THE PROGRAM AND ASK A PREVIOUS QUESTION (THIS ISN'T NECESSARY). IF THE ASKED IS ANY OTHER CHARACTER STRING BEGINNING WITH Q, THE SYSTEM THINKS THE PROGRAM IS TRYING TO READ A CONTROL CARD, AND ALLOWS NO FURTHER READS. IN THIS CASE, OR IF QEOF IS ENCOUNTERED AND NO EOF RETURN ADDRESS HAS BEEN SUPPLIED, THE PROGRAM PRINTS A SHORT MESSAGE AND EXITS.
ifstream profile (YES IO) ifstream

S(0) LIT *,
S(1) A4,S,
FLASH SA X11:RETURN *,
DS A1,SAVE * ,
DS A3,SAVE * ,
SR R1,SAVE * ,
SR R14,SAVE * ,
EXIT PACE * ,
LX X11:RETURN *,
LHJ L0.U A0.0742000 COMPARE TO JUMP INSTRUCTION,
L A0.0X11 GET ADDRESS OF USER'S QUESTION,
LHJ X11,ENDG AND INSERT IT INTO PRINT LINE,
LHJ X11,EDITX END EDIT MODE & RESTORE REGISTERS,
LHJ A0.3 INITIALIZE QUERY COUNTER,
ASK LHJ A0.0:REAMPRT * ,
READ LHJ A1:BLANKS * , FILL INPUT LINE WITH BLANKS SO THE,
LXJ U A2:1 * , PREVIOUS INPUT DOESN'T CONFUSE THE ISSUE,
LX4.U A2:INPUT * ,
LH+U R1.14 * ,
BT A2.0:*A1 * ,
LSL A0.6 *, DO A TREND TO PRINT QUESTION & GET ANSW.
JP A0,EXAMINE *, IS REPLY ACTUALLY IN 'INFO' FORMAT?
LA A0,REAMPRT+1, INPUT IS IN 'INFO' FORMAT...READ,
EXA READ * ,
EXAMINE LX1.U A2.0 *, INITIALIZE INDEX REGISTERS,
L+1 A3:INPUT * , IF FIRST CHARACTER IS NON-BLANK, SKIP,
L A0:INPUT * , TO SEARCHING FOR A MATCHING WORD,
TE U A3.5 *, 05 IS A BLANK,
J MATCH *,
LA A2:BLANKS *,
SHE A1:INPUT*A2 *, FIND FIRST WORD NOT ENTIRELY BLANK,
J AGAIN *, OOPS...THE WHOLE LINE HAS BLANK,
L A0:INPUT+1,A2 GET THAT FIRST NON-BLANK CHARACTER,
LHJ A3.5 *, FIGURE OUT WHICH CHARACTER IT IS,
LOOP A0:0700000000,090 MASK OUT LAST 5 CHARACTERS,
TE A1,0000000000U000 IS IT A BLANK,
J LOAD *, "10...00 LOOK FOR A MATCHING "ORL,
G LOAD A0.6 *, YES...TRY NEXT CHARACTER,
LSL A0.6 *,
J0D A3:LOOP * ,
LOAD DL A0,INPUT=1,A2 GET THE MESSAGE,
CJX MOVE+A3, SHIFT THE BLANKS AWAY,
LHJO U A2.0 *
MATCH LX-U R1.WCOUNCNT *, SEARCH FOR MATCHING WORD IN TABLE,
SE A0,TABLE=+A2 *,
J AGAIN *, NO MATCH...ASK AGAIN,
L A0,A2 FOUND A "MATCH"...GET INDEX,
LSL A0.35 LAST dIT IS 1 IF 'YES' 0 IF 'NO',
SSL A0.35, (SINCE A2 HAS BEEN INCREMENTED),
SLJ RESTORE *, RESTORE REGISTERS & RETURN,
TZ PRESENT *,
J 2X11 *, RETURN TO CALL+2 IF NO QEOF ADDR SUPPLIED,
J 3X11 *, RETURN TO CALL+3 SINCE QEOF ADDR PRESENT
****** PROFILE(YES,NO)******

Again L=U
A,U AGAINPKT
P"Y" Y"TTT"felt OR UTION ONLY ONE TIME
L=U
Again
L=U
EOF
J ASK
EOF
SLJ
RST
PKT
Present
QTH.
ONLY IF EOF reign simplified
WP
A,U+1
XI
Return to EOF address
L
A,U (IF EOF MTU RSTLIC")
EOF
EM
PRINTS
NON-EOF CONTROL CARD ENCOUNTERED...
EOF
EO
EXITS
WE'RE FORCED TO EXIT
PC
RESTORE RES 1
1 ROUTINE FOR RESTORING REGISTERS
PC
OL
SAVE
PC
OL
A,S
PC
OL
R1,SAVER
PC
OL
R14,SAVER
PC
OL
XI
XI
RETURN
PC
/
S(0)
PC
WR
EBCK
YES
NO
PC
15
RETURN
PC
16
SAVE RES 2
PC
17
SAVER RES 1
PC
18
SAVER1 RES 1
PC
19
PRESENT + -1
PC
20
PACKET ESPKT 24 LINE "YES", "NO", IF THE USER FORGETS THE STOP
PC
21
CHARACTER, A 0 IS THE CHARACTER MOST
PC
22
LIKELY TO BE FOUND BY ACCIDENT
PC
23
RSTLINE *CONTROL CARD FORCES PROGRAM EXIT*
PC
24
PRESENT EQU 3=RSTLINE *NUMBER OF WORDS IN MESSAGE
PC
25
PF FORM 12,6,1R
PC
26
READPKT PF 1,2=LINE+
PC
27
EOF
INPUT
PC
28
LINE RES 24
PC
29
AGAIN
EOF
PF 1,1=QUESTION
PC
30
EOF
INPUT
PC
31
QUESTION "WHAT?"
PC
32
INPUT RES 14
PC
33
BLANKS
PC
34
* THIS ENSURES THE SECOND WORD LOADED HAS
PC
35
* BLANK IF THE LAST WORD IN INPUT HAS INSTR,
PC
36
NOVE LDLS A0+30
PC
37
LJSL A0+12
PC
38
NUP
PC
39
TABLE *YES* EVEN RELATIVE LOCATIONS FOR "YES"
PC
40
"NO" OD FOR "NO"
PC
41
*Y*
PC
42
*Y*
PC
43
*Y*
PC
44
*Y*
PC
45
*Y*
PC
46
*Y*
PC
47
*Y*
PC
48
*Y*

ORIGINAL PAGE IS
OF POOR QUALITY
****** PROFILF (YESNO) ******

171  'YEA'   *
172  'NEIN' *,
173  'YES'   *
174  'NO'    *
175  'JA'    *
176  'NEIN' *
177  'DA'    *
178  'UNNE' *
179  'NEIN' *
180  'NEN' *,
181  'OK'    *
182  'NOT'   *
183  'OKAT' *
184  'N'     *
185  'S'     *
186  WACCOUNT EQU S-TABLE * THE NUMBER OF WORDS IN THE TABLE
187  END *

*N=EJECT
***** VPLT *****

20537JIN8D9KSPACE(1).VPLT
1 C NAME...
2 C VPLT
3 C
4 C PURPOSE...
5 C TO PRODUCE A PRINTERT-PILOT OF THE EXPERIMENTAL LINE PROFILE
6 C PRODUCED BY PROGRAM 'PROFILE'.
7 C
8 C USAGE...
9 C
10 C OPTIONS:
11 C
12 C QEOF
13 C
14 C
15 C
16 C
17 C
18 C
19 C
20 C
21 C
22 C
23 C
24 C
25 C
26 C
27 C
28 C
29 C
30 C
31 C
32 C
33 C
34 C
35 C
36 C
37 C
38 C
39 C
40 C
41 C
42 C
43 C
44 C
45 C
46 C
47 C
48 C
49 C
50 C
51 C
52 C
53 C
54 C
55 C
56 C

** NAME** VPLT

** PURPOSE** TO PRODUCE A PRINTERT-PILOT OF THE EXPERIMENTAL LINE PROFILE PRODUCED BY PROGRAM 'PROFILE'.

** USAGE**

OPTIONS:

QEOF

** INPUT**

DATA FILE AS PRODUCED BY PROGRAM 'PROFILE'

** SUBPROGRAMS REQUIRED**

BEGIN=OPT+NUMBER

** PARAMETER** LIMEXP=36

** LOGICAL** OPT,BATCH

REAL INT0,LENGTH,INTAV,IMAX,INCR,NL

DIMENSION LINE(105),HEADER(24),LENGTH(LIMEXP),INTAV(LIMEXP),SIG(LIMEXP)

DATA X1/"EOF/IMARA/I1"/,

CALL BEGIN('VPLT',1,2

IDIF:IONE-IZERO

** INPUT**

DATA FILE AS PRODUCED BY PROGRAM 'PROFILE'

SUBPROGRAMS REQUIRED...

BEGIN=OPT+NUMBER

** PARAMETER** LIMEXP=36

** LOGICAL** OPT,BATCH

REAL INT0,LENGTH,INTAV,IMAX,INCR,NL

DIMENSION LINE(105),HEADER(24),LENGTH(LIMEXP),INTAV(LIMEXP),SIG(LIMEXP)

DATA X1/"EOF/IMARA/I1"/

CALL BEGIN('VPLT',1,2

IDIF:IONE-IZERO

** FIND FILE AND READ FILE HEADER**

5 NFILE=NUMBER('FILE NUMBER',7:29,599)

DEFINE FILE 'FILE (14),1+3*LIMEXP+1*NREC

READ(IFILE')HEADER

39 C DECIDE WHICH IS ALL ('T' OPTION) OR LARGE GRAPH

ICOL=1

BATCH=NOT.OPT('Y')

IF BATCH)ICOL=101

COLOR=FLOAT(ICOL-1)

LAST=* *

IF BATCH)LAST=MARK

** READ A PROFILE**

8 IF(NREC.LE.14)GO TO 11

I=MAX(0,NREC-2)

10 PRINT 005

50 805 FORMAT(1X/13,* PROFILES)

PRINT 805

808 FORMAT(1H1)

GO TO 5

11 READ('FILE\NREC)INT0,LENGTH,INTAV,SIG

IF(INT0.EQ.0)GO TO 10

** SET UP SCALING PARAMETERS**
***** vPLUt *****

58 I'MAX=0.
59 NL=10.,
60 IF(LENGTH(IN)+1.LT. IC-5) OR (NL.NE.EXP)) GO TO 15
61 NL=NL+1
62 IF((NL.EQ.NL+1)NL=NL+1 LENGTH(I)-LENGTH(IN+1))
63 IMAX=IMAX+1, INTAV(I)+SIG(I))
64 NL=10.
65 IF((NL.LE.LENGTH(N)-LENGTH(I))LE. P4), AND. BATCH)NL=NL+2
66 NL IS NOT THE SCALE IN PRINT LINES PER ANGSTROM
67 TOTAL=NL*LENGTH(N)-LENGTH(I))
68 IF(TOTAL.GT.200.) GO TO 115
69 POWER=1.
70 IF(EQ.0) NL=NL-1.
71 POWER=POWER*10.
72 GO TO 20
73 IF(POWER*POWER.LE.10) GO TO 25
74 POWER=POWER*10.
75 N=NCAP+1
76 GO TO 20
77 IF(POWER.LE.10.) GO TO 30
78 POWER=POWER*10.
79 IFNCAP+1
80 GO TO 25
81 IF(POWER.LE.10.) GO TO 33
82 IF(POWER.LE.9.) GO TO 34
83 IF=10.
84 GO TO 40
85 NT=5
86 GO TO 40
87 NT=2
88 PRINT GRAPH HEADER
89 PRINT d10+HEADER:INTMON+FILE
90 FORMAT(111,12A6/IH
91 IF(POWER*POWER.LE.10) GO TO 33
92 POWER=POWER*10.
93 GO TO 25
94 PRINT TOP ORDER
95 DO 42 I=1,ICOL
96 LINE(I)=+*
97 LS=ICOL-1
98 DO 44 I=5,ICOL
99 LINE(I)=+*
100 PRINT d11,(LINE(I),J=1,ICOL)
101 PRINT d11 FORMAT(12TX,10SA1)
102 DO 44 I=5,ICOL
103 LINE(I)=+*
104 INSERT NEEDED BLANK LINES
105 DO 60 I=1,N
106 IF(SIG(I) .LT. 0.0) GO TO 60
107 LINES=IFIX(NL*LENGTH(I)-PREV)+5)
108 IF(LINES.GT.25) GO TO 50
109 IF(LINES.LE.1) GO TO 55
110 LINES=LINES-1
111 PRINT d12,MARK+LAST
****** VPLU T ******

812 FORMAT(27X,A1,9ymm A1)
114 UC TO 48
115 GO TO 48
116 56 PRINT 812,(MARK, LAST,I[1]+4)
117 PRINT 813 LAST
118 813 FORMAT(25X,\\\\\\\\\"**,**,T1P8,A1)
119 PRINT 812,(MARK, LAST,I[1]+4)
120 C
121 C
122 55 LINE(I)=MARK
123 LINE(I)=ICOL,LAST
124 J1=ICOL(INTAV(I)+SIG(I))
125 J2=ICOL(MAX(0,INTAV(I)-SIG(I)))
126 DO 57 J=J2+1
127 57 LINE(J)=**
128 PRINT 815,INTAV(I),SIG(I),LEN(I)
129 815 FORMAT(1X,F7.5,F7.5,F7.5,F7.5,F9.2,F14)
130 DO 59 J=J2+1
131 59 LINE(J)=**
132 60 CONTINUE
133 C
134 DO 62 I=1,ICOL
135 62 LINE(I)=**
136 DO 64 I=ICOL-1,1,-1
137 64 LINE(I)=**
138 PRINT 811,(LINE(I),J=1,ICOL)
139 DO 66 I=ICOL-1,1,-1
140 66 LINE(I)=**
141 C
142 DO 68 I=0,1
143 68 LINE(I+1)=ZERO+I,IDIF
144 IF(NOT.IDIF) GO TO 69
145 LINE(ICOL)=12"*RO
146 LINE(ICOL+1)=104E
147 69 IF(NP.LE.0,0,0) GO TO 70
148 LINE(ICOL+1)=*
149 LINE(ICOL+2)=*
150 LINE(ICOL+3)=*
151 IF(NP.LT.0)LINE(ICOL+3)=**
152 NCOL=ICOL+4
153 NCOL=ICOL+4
154 PRINT 811,(LINE(I),J=1,ICOL)
155 GO TO 70
156 GO TO 70
157 70 PRINT 811,(LINE(I),J=1,ICOL)
158 C
159 99 STOP
160 C
161 115 PRINT 915, TOTAL
162 915 FORMAT("**GRAPH LENGTH OR,**F6.0,** LINES IS TOO LONG!**)" GO TO 8
163 END
164 END
***** THEORY *****

NAME... THEORY

PURPOSE... TO FIND THE VALUES OF THE PARAMETERS (LINE POSITION, LINE INTENSITY, LINE WIDTH OR ELECTRON DENSITY, AND BACKGROUND INTENSITY) WHICH BEST FIT THE THEORETICAL PROFILE TO THE EXPERIMENTAL DATA.

USAGE... Q.THEORY OR QXOT .THEORY

DATA I IAGES:
CARD 1: (FREE) INPUT FILE 'NUMER
CARD 2: (FREE) OUTPUT FILE 'NUMFR, (ONLY WITH 'T' OPTION)
CARD 3: (FREE) WAVELENGTHS TO DELETE (ONLY WITH 'D' OPTION)
CARD 4: (FREE) LINL NUMBER
1 HE II 1640 (DENSITY 1.E17)
2 HE II 1215
3 HE II 1215
4 HE II 1022
5 HE II 606 (DENSITY 1.E17)
CARD 5: (FREE) YES' IF FIT TO THIS PROFtLE IS WANTED
ONLY WITH 'S' OPTION)
CARD 6: (FREE) 'YES' IF PLOT REQUESTED, 'NO' IF NOT
ONLY WITH 'D' OPTION)
(Repeat cards 5 & 6 FOR RAVING PROFILES AS NEEDED)

SUBPROGRAMS REQUIRED...

FETCHS OBTAINS THE 'NORMALIZED LINE PROFILE AND THEORETICAL LINE POSITION FOR THE LINE.
ZXPwL (FROM INS) GENERAL FUNCTION MINIMIZER, USED TO FIND THE NONLINEAR PARAMETERS WHICH MINIMIZE THE SUM OF THE SQUARES OF THE DEVIATIONS OF THE EXPERIMENTAL POINTS FROM THE THEORETICAL PROFILE.
FUNCT3 HAS THE THEORETICAL PROFILE CALCULATED FOR THE CURRENT PARAMETERS, AND OBTAINS THE MEAN SQUARE DEVIATION OF THE DATA FROM THE NEW PROFILE.
FUNCT2 FINDS THE CORRELATION MATRIX OF THE BEST-FIT PARAMETERS, USING THE SECOND PARTIAL DERIVATIVES OF THE ERROR FUNCTION.
IPLot PLTS THE EXPERIMENTAL DATA AND THEORETICAL PROFILE.
****** THEORY ******

#include UBANK
#include GROUP
#include /F3COM/ ARE2(2)
#include EXTERNAL Functions
#include REAL IAX
#include LOGICAL YESNO
#include KEEP
#include EXIT
#include IF(IF(LIF4EP*NE.O)PRINT 820
#include DFILC=tU'IBER(-IflPliT FILEQ,,7,29,$96)
#include OErI'd; FILE
#include OFILE(13,ISIZE,UOIITREC)
#include KEEP=.IJOT.OPT('lD'
#include IFC(fBAD.EO.O)(EEP=.TRUE.
#include CALL FETCHS(APGOIMALIIJE)
#include READ(DFILE)IIFT°-HEACER
#include PRINT 820.HEACER
#include FOR.4AT(IH112A6/1X.12A6)
#include LINEP=2
#include READ DATA FOR HFXT MONITOR INTFNSITY
#include READ(IF(File'DREC)BLOCK+NSHOT*LENGTH*INEXP
***** THEORY *****

104

C

DO 22 I=1,NARG
22 AR(I)=ARGW(I)

LINES(I)=LINE
IF(INI(I).GT.0.0.FND)GO TO 10

C CHECK FOR ACCEPTABLE WAVELENGTH RANGE

IF(ARG(2)+BASE.LT.2*LENGTH(I)-LENGTH(NU).OR.
- ARG(2)+BASE.GT.2*LENGTH(NU)-LENGTH(I)) GO TO 92

NU1=1
NU2=NU
IF(KEEP)GO TO 50

NU1=0
NU2=NU+1
38 NU1=NU1+1

IF(NU1.LE.NU2)GO TO 49

DO 40 I=1,IAB
40 CONTINUE

IF(ARGCZ)+BASE.LT.ZSLNGTH(t)-LENGTH(NU)) OR.
U ARG62)*BASE.GT.2sLEIGTH(NU)-LENGTH()) G TO 92

NU1=1
NU2=NU
IF(KEEP)GO TO 50

NU1=0
NU2=NU+1
47

IF(NU1.LE.NU2)GO TO 49

DO 40 I=1,IAB
40 CONTINUE

NU1=NU1+1
NU2=NU+1

IF(NOI.oE.4U2)GO TO 40

DO
44 I=INBAV
45 CONTINUE

IF(ALSCLENGTII(NU2)-BAD(Z)).LT. .001)GO

CONTINUE

GO TO 42

NU2=NU1
NU2=NU2-1

IF(NOI.oE.4U2)GO TO 40

DO
44 I=INBAV
45 CONTINUE

IF(ALSCLENGTII(NU2)-BAD(Z)).LT. .001)GO

CONTINUE

GO TO 42

IF(ALSCLENGTII(NU2)-BAD(Z)).LT. .001)GO

CONTINUE

GO TO 42

IF(ALSCLENGTII(NU2)-BAD(Z)).LT. .001)GO

CONTINUE

GO TO 42

HOLD=LENGTH(NU1)
LENGTH(NU1)=LENGTH(NU2)
LENGTH(NU2)=HOLD

NS=MAX(NSHOT(NU1)+NSHOT(NU2))
NSHOT(NU1)=NS
NSHOT(NU2)=NS
GO TO 39

49 NU2=NU

PRINT LABEL8 INFORMATION

50 TOTAL=0
51 BOTTOM=LENGTH(NU1)
TOP=LENGTH(NU2)
AVG=0.

53 DO 51 K=1,NU
54 BOTTOM=BOTTOM+NU(K)
55 TOTAL=TOTAL+NU
56 A=AVG+INEXP(KU)+KSHOT

58 TOP=A+AX1(TOP+LENGTH(KU))
59 NSHOT(KU)=NS
60 TOTAL=TOTAL+A
61 DO 51 KSHOT=KU

51 AVG=AVG+INEXP(KU)+KSHOT
AVG=AVG/TOTAL

63 IF(AVG.LT.1.E-5)GO TO 95

65 LEP=LINEP+13

66 IF(LENGTH(LT)-3)GO TO 53

67 PRINT 260,HEADER
LINEP=15
69 PRINT 830,TERM+TOTAL+BOTTOM+TOP
830 FORMAT(1X/ TIME**,F6.3,**MONITOR**,F6.4/)
**THEORY**

171 - $1x^{1.5}$, $0.1x^{1.5}$, $\text{AVALE}^{0.5}$, $F_{p2}$, $F_{0}$
172 IF (ALL GO TO 65
173 IF (F111$, F111$, F211$, 0.96) GO TO 55
174 LINESLINES=11
175 GO TO 20
176 C 55 I=NU2-NU1+1
177 IF (I.E. ARG2*2) GO TO 93
178 C SET UP FOR SOLUTION
179 C NEVAL=0
180 DO 60 ITER=1,6
181 A1=ARG(1)
182 ARG2(1)=9.9
183 ARG2(2)=9.9
184 CALL HESS(ARG2,ARG)
185 LI4=11
186 C HAVE MINIMUM FOUND (USING ROUTINE FROM IMSL)
187 CALL ZPOLL(FUNCTION,CLOSE,ARG,VALUE,LIMIT,IER)
188 IF(OUT,11) 760,ARG(1),ARG(2),VALUE,IER
189 760 FORMAT(*) RESULTS: *.3G,13,14)
190 C IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
191 IF (A5(ARG(1)-A1) *L.T. +1*ARG(1)) GO TO 65
192 CONTINUE
193 IF (OUT) 638,ITER=1
194 638 FORMAT(*) DENSITY DID'NT CONVERGE AFTER 14 ITERATIONS, HAVE"
195 - $1$EIP=13)
196 C REPEAT WITH CLOSER TOLERANCES
197 60 CONTINUE
198 CONTINUE
199 CALL HESS(ARG2,ARG)
200 CALL ZPOLL(FUNCTION,CLOSE,ARG,VALUE,LIMIT,IER)
201 IF (VALUE LT. 0.01*EST) GO TO 94
202 C IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
203 IF (A5(ARG(1)-A1) *L.T. +1*ARG(1)) GO TO 65
204 C UPDATE ESTIMATE OF MINIMUM VALUE
205 C FIX ERRORS IN CALCULATED PARAMETERS
206 C CALL FUNCT2
207 C PRINT RESULTS
208 PRINT 810,ITER,NEVAL,IER,WIDTH,FP,VALUE
209 810 FORMAT (*) ITERATION=$S$1$,1S$1', EVALUATION=$S$1',1S$1, ERROR CODE: $S$1
210 C IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
211 C IF (A5(ARG(1)-A1) *L.T. +1*ARG(1)) GO TO 65
212 C UPDATE ESTIMATE OF MINIMUM VALUE
213 C CALL FUNCT2
214 C PRINT RESULTS
215 PRINT 846,ITER,NEVAL,IER,WIDTH,FP,VALUE
216 846 FORMAT (*) ITERATION=$S$1$,1S$1', EVALUATION=$S$1',1S$1, ERROR CODE: $S$1
217 C 1S$1',1S$1
218 C IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
219 C IF (A5(ARG(1)-A1) *L.T. +1*ARG(1)) GO TO 65
220 C UPDATE ESTIMATE OF MINIMUM VALUE
221 C CALL FUNCT2
222 C PRINT RESULTS
223 C IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
224 C IF (A5(ARG(1)-A1) *L.T. +1*ARG(1)) GO TO 65
225 C UPDATE ESTIMATE OF MINIMUM VALUE
226 C CALL FUNCT2
227 C PRINT RESULTS

**ORIGINAL PAGE IS OF POOR QUALITY**
***** DIARY *****

228 PRINT 447; 'T(I),E(I),I1,COVX(I),I2(COVX(I),I2)
229 647 FORMAT (T(I),E(I),I1,COVX(I),I2)
230 IF(PLTOUT.EQ.T),E.T(2))
231 PRINT 840,INT(2),E(2),INT(1),COVX(1),INT(4)
232 648 FORMAT(' BACKGROU D INTENSITY='F7.4,'='F6.4;10,'='T7.3F6.2)
233 - (F6.2)
234 IF(RATIO.LT.1.E-5) GO TO 70
235 I=IPCENT(RATIO(I)/RATIO(I))
236 PRINT 350,RATIO(I),EXATIO(I),I1
237 850 FORMAT(T110,T13;LINECONTEN=T,F7.2,'=',F6.2;16,'F7.4')
238 IF LINE IS HE II 4686, FIND 6 PRINT TEMPERATURE
239 IF(ARGS(2).LT.-4695.766) GO TO 70
240 I=IPCENT(TEMP/TEMP)
241 PRINT 855,TEMP,TEMP+11
242 855 FORMAT(T111;TEMPERATURE='F7.2'='F6.2;16,'F7.4')
243 LINEP=LINEP+1
244 WRITE RESULTS TO FILE IF DESIRED
245 IF(OUTF) WRITE(OUT1,OUT1) BLOCK, K1, LENGTH, INEXP
246 ARG(1)=1.E-16*ARG(1)
247 PLOT NO IF DESIRED
248 IF(LATER) GO TO 20
249 LINEP=LINEP+1
250 IF(.NOT.ONEPLOT(1,596)) GO TO 20
251 CALL PLOT(MAX(OUTTOP),TOP)
252 PRINT 850,MAX(OUTTOP),TOP
253 860 FORMAT('AXIS LABELS='F7.4;2F8.1)
254 LINEP=LINEP+1
255 GO TO 20
256 VERIFY OF ERRORS
257 260 A=AABS+ARG(2)
259 902 FORMAT('LINE CENTER OF='F9.2,' TOO FAR FROM EXP RANGE='F9.2)
260 = TO='F9.2)
261 GO TO 90
262 901 PRINT 903,1
263 903 FORMAT(16,'(0LMT,'I2,9' POINTS PRESENT')
264 GO TO 96
265 904 PRINT 904
266 904 FORMAT('SIGMA SQUA RDED IS TOO SMALL')
267 A=A=AABS+ARG(1)
268 S20
269 PRINT 840,IVector,EVAT,VALUES,A+S
270 A=ARG(2)+BASE
271 PRINT 840,LABEL(LINES,LINES),LABEL(LINES)+S
272 GO TO 20
273 95 PRINT 905,AVG
274 905 FORMAT('SIGNALS AVERAGE ONLY='F15.6,'')
275 GO TO 20
276 96 IF(OUTAND.OUTREC,L1) WRITE(OUTFIL,OUTREC) END
277 STOP
278 97 PRINT 907,INF;TFMT
279 907 FORMAT(' INPUT DATA FILE FORMAT IS='F7,' RATHER THAN='F4')
280 STOP
281 END
****** THEORY (MA1) ******

20537J1.MATK5 &GSPACE(J2),GJM
1 D8AIK PROC
2 C
3 C     PROCEDURE NAME...
4 C     D8AIK
5 C
6 C     PURPOSE... TO TRANSMIT THEORETICAL, EXPERIMENTAL, AND CALCULATED
7 C     INFORMATION PAST THE LIBRARY ROUTINE *FMCG*
8 C
9 C
10 C     PROGRAMS USING THIS PROCEDURE...
11 C
12 C
13 C     FETCHS*FUNCTION*NEW1,NEW2,NEW3,NEW4,SIGMA,SUM,THEORY,TPLOT
14 C
15 C
16 C     PARAMETER LVMC=10
17 C     PARAMETER LINES=38
18 C     CHARACTER LINES=8B
19 C     INTEGER TOTAL
20 C     LOGICAL OPT
21 C     REAL LINES(10),CNST
22 C     COMMON K5,KU(5),N2,SHOT,TOTAL,NEW1,ITER,ITER,LP5,LP5,UX2,LX2,UX1,LX1,
23 C     SIG(4),INT(4),ERROR(4),ERROR(4),COVAR(4,4)
24 C
25 C     EQUIVALENCE (RLOCK(1),INT1)
26 C     END

****** THEORY (GROUP) ******

20537J1.MATK5 &GSPACE(J2),GJM
1 GROUP PROC
2 C
3 C     PROCEDURE NAME...
4 C     GROUP
5 C
6 C     PURPOSE... TO COMMUNICATE PARAMETER ERROR ESTIMATES.
7 C
8 C     PROGRAMS USING THIS PROCEDURE...
9 C
10 C     THEORY,FUNCTION
11 C
12 C     PARAMETER LINES=38+(2*LINES)+LINES
13 C     COMMON/GROUP/ INTMON+TAVER+NU1+NU2+HARG+TEMP+ETEMP,
14 C     LINES(10),
15 C     VALUE+WIDTH,
16 C     ARG(4)+SIG(4)+INT(4)+RATIO(3)+RATIO(3)+COVAR(4,4)
17 C     DIMENSION ULOCK(55)
18 C     EQUIVALENCE (RLOCK(1),INT1)
19 C     END

ORIGINAL PAGE IS OF POOR QUALITY
**** THEORY (FETCHS) ****

SUBROUTINE FETCHS(ARG,NARG,LINES)

NAME...

PURPOSE...

TO DETERMINE WHICH LINE HAS BEEN SCANNED, READ IN THE
CORRESPONDING THEORETICAL PROFILE, AND INITIALIZE THE
NONLINEAR PARAMETERS.

CALLING SEQUENCE...

CALL FETCHS (ARG,NARG,LINES)

ARG R0

ARRAY OF NONLINEAR PARAMETERS

ARG(1) IS THE ELECTRON DENSITY TIMES 1.E-16.

ARG(2) IS THE DISTANCE FROM THEORETICAL

TO ACTUAL LINE CENTER.

NARG I0

NUMBER OF NONLINEAR PARAMETERS

LINES I0

LINE COD NUMPER.

1 HE II 4686 (DENSITY 1.E17)

2 HE II 1080

3 HE II 1215

4 HE II 1025

5 HE II 4686 (DENSITY 1.E18)

VARIABLES IN BLANK COMMON:

NARG I0

NUMBER OF NONLINEAR ARGUMENTS

NS1=NS2

# ENTRIES IN ARRAYS ALPH1, SALPH1 AND

ALPH2, SALPH2, RESPECTIVELY

HHW R0

HALF HALF WIDTH OF 1STRUMENT FUNCTION

BASE R0

THEORETICAL LINE CENTER MINUS 10 ANGSTROMS

ALPH1+SALPH1

ARRAYS OF VALUES OF ALPHA & SALPHA

INCLUE DBNKL, LIST

DIMENSION ARG(4)

INTEGER STHEO

LOGICAL OPT

DATA STHEO/29/*IFMT/000/

DEFINE FILE STHEO/I02*LINES+1*IFMT+1*

READ(STHEO+1)*PHI

IF(NIPF.THE+1*IFMT+10 TO 90

NARG=2

START WITH AN ELECTRON DENSITY OF 10**17

ARG(1)=1.E-16+1.E17

LINES=NUMBER*LINE NUMBER*1.9*30

READ(STHEO+1)LINES+1*BASE+ALPH1+SALPH1

NS1=1

NS2=NS1+1

ARG(2)=10.

BASE+BASE=10.

IF(BASE.LT.3000)GO TO 25

HHW=3
****** THEORY (FLTSHS) ******

57 IF(OPT('C'))$H$W=ax001
58 RETURN,
59 25 $ASE=ase=.58
60 $H$W=ax334
61 IF(OPT('C'))$H$W=ax001
62 RETURN
63 30 STOP
64 90 PRINT 904,IFMT,IFMT
65 90A FORMAT('$(ALPHA) FILE FORMAT IS 15,15,' RATHER THAN',14)
66 STOP
67 END

*** END
**** THEORY (FUNCT3) ****

FUNCTION FUNCT3 (ARG)

PURPOSE

TO FIND THE MEAN SQUARE DEVIATION OF THE DATA FROM THE

THEORY USING CURRENT PARAMETERS.

INCLUDE UBANK,List
INTEGER IJCT3/0/
DIMENSION ARG(1)
LOGICAL OPT
COMMON/FACOM/A(2),+10,VO,LO,NF

IF(A(1).NE.ARG(1)).OR.A(2).NE.ARG(2))

- ANGLE=S7.296*(ARG(2)-A(1),ARG(1)-A(1))

IF(AHS(A(2)-0).GT.26).LWCT=ENRCT+1

IF(AHS(A(2)-1).LT.-1.E-7*ARG(1))GO TO 10

IF(A(I).LT.1. OR. A(I).GT.1000.0)ERRCT=ERRCT+1

IF(ERRCT.GE.8)GO TO 90

IF(BRIGHT. LT. -1.E-5)GO TO 90

CALL I/UCT(ARG(2))

A(I)=A(I(1))

10 CALL IJUCT(ARG,2)

FUNCTION=SIGCA(ARG)

IF(ANGLE.LE.0.1)ANGLE=ANGLE+100.

IF(OPT('Z').AND. ABS(ANGLE-OLDA).GT.4)

- PRINT 703,A,OLDA,

IF(OPT('X'))

- PRINT 701;A(1),A(2),FUNCT3,ANGLE,BRIGHTBACKGO

701 FORMAT(3415.6,F5.0,IP59.31

A(2)=ARG(2)

OLDA=FUNCT3

OLDA=NGLE

NEVAL=NEVAL+1

RETURN.

90 PRINT 703

703 FORMAT(****FUNCT3** FINDS SURFASOMABLE ARGUMNENTS (BTI TIME).))

PRINT 701,A,OLDA,OLD=NG

PRINT 707;ARG(1)BASE,ARG(2),FMT=BRIGHTBACK0

707 FORMAT('**FMT (I): 1); =MLBE+1ARG+3; ;CFMT+69.5,*,613.6,*, FMT=*

- >999,J;RIIGHTAIFDS(5),209,3)

D0 92 KUMUL.L/NP

XX=XX+1(1)

YY=NVALUE(DEL+TOEL*VS2,XX+BASE-ARG(2),/)

Y2=0.

92 DO 92 KUMUL.L/NP

AX=XX+I(KU)

YY=VALUE(DEL+TOEL*VS2,XX+BASE-ARG(2),/)

Y2=0.

M=NSHOT(KU)

D0 91 KUMUL.L/NP

Y2=YS#1

92 PRINT 724,XX,Y2,YY

724 FORMAT(1PG14.6,2Il.2)

STOP

END
*** THFURY (FUNCT2) ***

20573Jul#OKB#ACES(1).FUNCT2
SUBROUTINE FUNCT2

NAME...
FUNCT2

PURPOSE...
TO FIND THE EXPECTED ERRORS IN THE FIRST-FIT PARAMETERS.

CALLING SEQUENCE...

CALL FUNCT2

VARIABLES IN BLANK COMMON:

TOTAL I+1 # DATA POINTS
EPSI R+1 STEP IN WAVELENGTH
EPSNE R+1 STEP IN ELECTRON DENSITY = ARG(1)
FO R+0 HOLOGRAM FIELD STRENGTH
JASE R+1 THEORETICAL LIFE CENTER MINUS 10 ANGSTROMS

VARIABLES I' COMMON /GROUP/

NARG I+1 NUMBER OF ELEMENTS IN ARG
ARG R+1 ARRAY OF NONLINEAR PARAMETERS
VALUE R+10 INPUT: SUM OF SQUARES OF DEVIATIONS
FOR THE FIRST-FIT PARAMETERS. OUTPUT: SQUARE ROOT OF SUM OF SQUARES.
SIG R+0 ARRAY OF EXPECTED ERRORS IN THE NONLINEAR PARAMETERS
LIT R+0 ARRAY OF LINEAR PARAMETERS
E R+0 ARRAY OF EXPECTED ERRORS OF LINEAR PARAMETERS
COVAR R+0 UPPER TRIANGLE IS SET TO A NORMALIZED VARIANCE-COVARIANCE MATRIX.
RATIO R+0 LINE TO (100 ANGSTROM) CONTINUUM RATIO
ERATIO R+0 EXPECTED ERROR IN RATIO
TEMP R+0 TEMPERATURE FROM THE LINE/CONTINUUM RATIO
ETEMP R+0 EXPECTED EXPERIMENTAL ERROR IN TEMP
WIDTH R+0 HALF HALF WIDTH OF EXPERIMENTAL LINE (ANGSTROMS)

METHOD...
THE VARIANCE-COVARIANCE MATRIX IS NORMALIZED BY DIVIDING EACH ROW AND EACH COLUMN BY THE SQUARE ROOT OF THE ORIGINAL DIAGONAL ELEMENT, THE CALCULATIONS OF FRATIO AND ETEMP MAKE USE OF THE APPROXIMATELY KNOWN COVARIANCE MATRIX ELEMENTS.
THE TEMPERATURE IS FOUND USING THE THEORETICAL RESULTS OF DELORIX AND VOLKITE.

SUBPROGRAMS REQUIRED...

NEWTON/SUM/F/SLMN/S/MIN

DIMENSION ARGUM(4)
LOGICAL OPT
DIMENSION TATTLE(6)

ORIGINAL PAGE IS OF POOR QUALITY
****** THEORY (FUNCTION2) ******

DATA *SIGMA/10.0, SIGMA/10.0/
REAL INT
INCLUDE JAVANLIST
INCLUDE GROUPLIST
GET THE FINAL VALUES OF THE SUM OF SQUARES & ERROR

C
MATRIX ELEMENTS

CALL NEWT(ARG,NARG)
CALL NEWT(ARG,NARG)
V1=SIGMA(ARG)
IF(OPT('O')*)PRINT 701,ARG(1),ARG(2),V1

701 FORMAT(0 ' 2G13.6* ' I4*G12.6)
V1=SUMF(ARG)
IF(OPT('O')*)PRINT 701,ARG(1),ARG(2),V1
MARKER
BEPSI+SIGMA*EPSI
BEPSI=SIGMA*EPSI
DO 10 I=1,NARG
10 ARGUM(I)=ARG(I)
CALL SUMF(ARGU,NARG)
CALL SUMF(ARGU,NARG)
V1=SIGMA(ARGU)
IF(S1.LT.VALUE)MARKER=1

11 CALL NEWT(ARG1,NARG)
12 CALL NEWT(ARG1,NARG)
13 S1=SIGMA(ARGU)
14 IF(S1.LT.VALUE)MARKER=1
15 TATTLE(4)=S1
16 ARGU(2)=ARG(2)+BEPSI
17 CALL SUMF(ARGU,NARG)
18 IF(S2.LT.VALUE)MARKER=1
19 TATTLE(5)=S2
20 COVAR(2,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
21 ARGU(1)=ARG(1)+BEPSI
22 CALL NEWT(ARGU,NARG)
23 S1=SIGMA(ARGU)
24 IF(S1.LT.VALUE)MARKER=1
25 TATTLE(4)=S1
26 ARGU(1)=ARG(2)
27 CALL SUMF(ARGU,NARG)
28 IF(S2.LT.VALUE)MARKER=1
29 TATTLE(5)=S2
30 COVAR(2,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
31 ARGU(1)=ARG(1)+BEPSI
32 CALL NEWT(ARGU,NARG)
33 S1=SIGMA(ARGU)
34 IF(S1.LT.VALUE)MARKER=1
35 TATTLE(4)=S1
36 ARGU(1)=ARG(1)
37 CALL SUMF(ARGU,NARG)
38 IF(S1.LT.VALUE)MARKER=1
39 TATTLE(4)=S1
40 IF(MARKER.EQ.1)PRINT 702
41 702 FORMAT(1 ' 4X,9F13.6/3613.6/13X.613.6/13X.6/3613.6/13X.6')
42 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
43 ARGU(1)=ARG(1)-BEPSI
44 CALL NEWT(ARGU,NARG)
45 TATTLE(4)=S1
46 IF(MARKER.EQ.1)PRINT 702
48 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
49 ARGU(1)=ARG(1)-BEPSI
50 CALL NEWT(ARGU,NARG)
51 S1=SIGMA(ARGU)
52 IF(S1.LT.VALUE)MARKER=1
53 TATTLE(4)=S1
54 IF(MARKER.EQ.1)PRINT 702
56 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
57 ARGU(1)=ARG(1)-BEPSI
58 CALL NEWT(ARGU,NARG)
59 TATTLE(4)=S1
60 IF(MARKER.EQ.1)PRINT 702
62 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
63 ARGU(1)=ARG(1)-BEPSI
64 CALL NEWT(ARGU,NARG)
65 TATTLE(4)=S1
66 IF(MARKER.EQ.1)PRINT 702
68 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
69 ARGU(1)=ARG(1)-BEPSI
70 CALL NEWT(ARGU,NARG)
71 TATTLE(4)=S1
72 IF(MARKER.EQ.1)PRINT 702
73 702 FORMAT(1 ' 4X,9F13.6/3613.6/13X.613.6/13X.6/3613.6/13X.6')
74 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
75 ARGU(1)=ARG(1)-BEPSI
76 CALL NEWT(ARGU,NARG)
77 TATTLE(4)=S1
78 IF(MARKER.EQ.1)PRINT 702
80 COVAR(1,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
81 ARGU(1)=ARG(1)-BEPSI
82 CALL NEWT(ARGU,NARG)
83 S1=SIGMA(ARGU)
84 IF(S1.LT.VALUE)MARKER=1
85 TATTLE(4)=S1
86 ARGU(2)=ARG(2)+BEPSI
87 CALL SUMF(ARGU,NARG)
88 IF(S2.LT.VALUE)MARKER=1
89 TATTLE(5)=S2
90 COVAR(2,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
91 ARGU(1)=ARG(1)+BEPSI
92 CALL NEWT(ARGU,NARG)
93 S1=SIGMA(ARGU)
94 IF(S1.LT.VALUE)MARKER=1
95 TATTLE(4)=S1
96 ARGU(2)=ARG(2)+BEPSI
97 CALL SUMF(ARGU,NARG)
98 IF(S2.LT.VALUE)MARKER=1
99 TATTLE(5)=S2
100 COVAR(2,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
101 ARGU(1)=ARG(1)+BEPSI
102 CALL NEWT(ARGU,NARG)
103 S1=SIGMA(ARGU)
104 IF(S1.LT.VALUE)MARKER=1  
105 TATTLE(4)=S1
106 IF(MARKER.EQ.1)PRINT 702
108 - ' FOLLOW ******'
109 IF(MARKER.EQ.1 .OR. OPT('O'))PRINT 707 TATTLE
110 707 FORMAT(13X,2G13.6/3613.6/13X.613.6/3613.6/13X.6)
111 COVAR(1,1)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
112 COVAR(1,3)=(SFD3-SFD)/BEPSI
113 COVAR(1,4)=(SFD3-SFD)/BEPSI
****** THEORY (FUNCTION) ******

114       COVAR(1,2)=1.E63*COVAR(1,2)/SIG(1)
115       COVAR(1,3)=1.E63*COVAR(1,3)/SIG(1)
116       COVAR(1,4)=1.E63*COVAR(1,4)/SIG(1)
117       COVAR(2,3)=1.E63*COVAR(2,3)/SIG(2)
118       COVAR(2,4)=1.E63*COVAR(2,4)/SIG(2)
120       C INTEGRAL TO FIND THE VARIANCE-COVARIANCE MATRIX
121 15 IF(0.01>PRT0.001)PRINT 715,(COVAR(I,J),I=1,J)
122 715 FORMAT(1X,4G13.6)
123       CALL SYMINV(COVAT=4*G4*00+B0)
124       DO 25 J=1,4
125 18 IF(0.01>PRT0.001)PRINT 715,(COVAR(I,J),I=1,J)
126       DO 20 J=1,4
127 20 COVAR(I,J)=COVAR(I,J)+
129       C RESCALE ELECTRON DENSITY
130       ARG(1)=1.E6*ARG(1)
131       C CORRECT REFERENCE TO DENSITY
132       C DENSITY ACTUALLY VARIES LIKE (LINE 40)DI**1.2
133       R=1.35
134       IF(ABS(ARG(2)+BASE-40T5.75).GT.10.)GO TO 25
135       R=1.35*ARG(1)/1.5
136       ARG(1)=1.35*ARG(1)/1.5
137       C WE MUST RECALCULATE THE HOLTSMAN FIELD STRENGTH
138 160 IF THE LINE COINCIDENCE RATIO & ERROR
139       RATIO=INT(1)/(INT(2)*10.)
140       ERROR=RATIO**2
141       C EXTRACT THE VARIANCES OF THE INDIVIDUAL PARAMETERS
142 156 IF LINE IS NOT 45.75, FIND TEMPERATURE & ERROR
143       IF (RATIO.LT..01) OR (ABS(ARG(2)+BASE-40T5.75).GT.10.)GO TO 30
144       TR=2.05*ABS(ARG(2)+BASE-40T5.75)+2.05*ABS(ARG(1)-40T10)
145       T=(2.05*ABS(ARG(2)+BASE-40T5.75)+2.05*ABS(ARG(1)-40T10))**5.10
146       TC=9.99/INT(2)
147       C TEMP=SORTABS(T/INT(T)*COVAR(11))
148       C TEMP=SORTABS(T/INT(T)*COVAR(11))
149       C TEMP=SORTABS(T/INT(T)*COVAR(11))
150       C TEMP=SORTABS(T/INT(T)*COVAR(11))
151       C TEMP=SORTABS(T/INT(T)*COVAR(11))
152       C TEMP=SORTABS(T/INT(T)*COVAR(11))
153       C TEMP=SORTABS(T/INT(T)*COVAR(11))
154       C TEMP=SORTABS(T/INT(T)*COVAR(11))
155       C TEMP=SORTABS(T/INT(T)*COVAR(11))
156       C TEMP=SORTABS(T/INT(T)*COVAR(11))
157       C TEMP=SORTABS(T/INT(T)*COVAR(11))
158       C TEMP=SORTABS(T/INT(T)*COVAR(11))
159       C TEMP=SORTABS(T/INT(T)*COVAR(11))
160       C TEMP=SORTABS(T/INT(T)*COVAR(11))
161       C TEMP=SORTABS(T/INT(T)*COVAR(11))
162       C TEMP=SORTABS(T/INT(T)*COVAR(11))
163       C TEMP=SORTABS(T/INT(T)*COVAR(11))
164       C TEMP=SORTABS(T/INT(T)*COVAR(11))
165       C TEMP=SORTABS(T/INT(T)*COVAR(11))
166       C TEMP=SORTABS(T/INT(T)*COVAR(11))
167       C TEMP=SORTABS(T/INT(T)*COVAR(11))
168       C TEMP=SORTABS(T/INT(T)*COVAR(11))
169       C TEMP=SORTABS(T/INT(T)*COVAR(11))
170       C TEMP=SORTABS(T/INT(T)*COVAR(11))

ORIGINAL PAGE IS OF POOR QUALITY.
***** THEORY (FUNCT2) *****

171 COVAR(1*4)=COVAR(1*4)/([SIG(1)*E(1)]
172 COVAR(3*4)=COVAR(3*4)/([SIG(3)*E(2)])
173 DO 40 J=1,4
174 40 COVAR(J,J)=1.
175 C FIND HALF INTENSITY POINT OF EXPERIMENTAL PROFILE
176 HALF=DEL(2)/2.
177 DO 45 K=2,N52
178 IF(DJLL(KS).LT.HALF) GO TO 49
179 45 CONTINUE
180 KS=N52
181 X1=DEL(KS)
182 X2=DEL(KS-1)
183 Y2=DEL(KS-1)
184 DO 54 J=1,4
185 X=(Y2-HALF)*X1-(Y1-HALF)*X2)/(Y2-Y1)
186 X1=X
187 Y2=Y1
188 50 Y1=VALUE(DEL,DEL,NS2,X1)
189 51 WIDTH=((Y2-HALF)*X1-(Y1-HALF)*X2)/(Y2-Y1)
190 52 VALUE=SQRT(V)
191 RETURN
192 60 PRINT 908
193 908 FORMAT(' INVERSION FAILURE FINDING COVARIANCE MATRIX')
194 RETURN
195 END

W.EJLT
****** THEORY (TPLOT) ******

SUBROUTINE TPLLOT(YMAX,BOTTOM,TOP)

NAME***

TPLLOT

PURPOSE***

TO PLOT THE EXPERIMENTAL DATA AND THEORETICAL BEST

FIT PROFILE.

USAGE***

CALL TPLLOT (YMAX,BOTTOM,TOP)

AMAX R+0 LABEL FOR END OF Y AXIS

BOTTOM R+0 LABEL FOR ORIGIN OF X AXIS

TOP R+0 LABEL FOR END OF X AXIS

VARIABLES IN COMMON: ALMOST EVERYTHING

SUBROUTINES USED...

PLOTC STANDARD PLOT SUBROUTINE, USED TO POSITION THE PEN

NSCALE FILL'S PLOT SCALING PARAMETERS FOR EASILY INTERPRETED

AXIS LABELS

AXIS DRAWS AN AXIS

'SYMBOL' PLANS A SYMBOL AT THE DESIRED POSITION

PAGEUP COMPLETES THE PLOT AND POSITIONS THE PEN ONTO

THE NEXT PAGE

METHOD***

NOTE THAT THE AXES USED IN THIS ROUTINE ARE ROTATED 90

DEGREES CCW FROM THOSE USED BY THE SYSTEM ROUTINES. THIS:

MY Y+ DIRECTION IS THEIR X-, AND MY X+ DIRECTION IS THEIR X+.

DIMENSION ARG(4),INT(4)

INCLUDE OBANK,LIST

INCLUDE GROUP,LIST

REAL L,X(1),LROW

DATA WIDTH,HEIGHT, NY, NX

/ 8:* 5:5, 5 15/*

C

FIT(Z)=INT(1)*VALUE(DEL,DEL+52+Z0)*INT(NAPG)

C

FIND LARGEST & SMALLEST VALUES ALONG EACH AXIS

BOTTOM=LENGTH(1)

TOP=LENGTH(NU)

YMAX=FIT(0)

CENTER=ARG(2)+BASE

UBOUND=CTCTER+10.+WIDTH

LBOUND=CTCTER-10.+WIDTH

DO 15 KU=1,NU

15 CONTINUE

DOUOT PLOT POINTS FURTHER THAN 10 HW TO EITHER SIDE

IF(LENGTH(KU),GE,UBOUND)BOTTOM=AMAX(BOTTOM,LENGTH(KU))

IF(LENGTH(KU),LE,LBOUND)TOP=AMAX(TOP,LENGTH(KU))

NNSHOT(KU)
***** THEORY (T PLOT) *****

DO 10 K=1,N

10 YMAX=MAX1(YMAX,INTERP(KU+KSHOT))
C PLOT AT LEAST 4 MPH TO EACH SIDE
BOTT =A MIN1(BOTT+CLTEN+G.,*MIN1)$
TOP=APAX1(TOP+CENTR+4.*MIN1)
C FIND SCALING PARAMETERS
NTICX=NX
CALL NSCALE(BOTT+TOP+NTICX+WIDTH,DX)
DX=1./DX
NTICY=NY
ZERO=0.
CALL NSCALE(ZERO,YMAX,NTICY,HEIGHT,DY)
DY=1./DY
C CALL PLOTC(7.5,1.0,0,-3)
C CALL PLOTC(U,LZ,3)
C CALL PLOTC(U,L+DLZ)
18 L=L+UL+DLZ
C DRAW THE THEORETICAL CURVE
L=TOP
DLZ=TOP-BOTTOM)/250.
NPEN=3
DO 40 KU=1,251
C CALL PLOTC(DY*UL+DLZ,NPEN)
NPEN=2
40 L=L+DLZ
C DRAW A DOTTED LINE FOR THE CONTINUUM LEVEL
C (IF POSITIVE)
IF(INT(NARG)+L.T.0.)GO TO 20
U=INT(INT(NARG)
L=DX*(TOP+BOTTOM)
DL=L/69.
DO 18 KU=1,35
CALL PLOTC(U,L+3)
18 CALL PLOTC(U,L+DL)
C PLOT THE EXPERIMENTAL POINTS
C IF(KU.EQ.KU2)SYMP=0
IF(LNGTH(KU).LT.BOTTOM .OR. LNGTH(KU).GT.TOP) GO TO 30
U=0.
KSHOT=1.N
DO 25 KSHOT=1.N
25 CALL SYMC(UL+DLZ,Lngth(KU)-BOTTOM)*.1+NSTMB,96**1)
30 IF(KU.EQ.KU2)SYMB=4
C DRAW AXES
CALL AXISN(O.,O.,NTICY HEIGHT-.1,180.)
CALL AXISN(O.,G..NTICX WIDTH,.1,90.)
C DRAW AXES
CALL PLOTC(U,L,3)
C PLOT THE EXPERIMENTAL POINTS
C (IF POSITIVE)
DO 30 K=1,N
C IF(KU.EQ.KU2)SYMP=0
IF(LNGTH(KU).LT.BOTTOM .OR. LNGTH(KU).GT.TOP) GO TO 30
U=0.
KSHOT=1.N
DO 25 KSHOT=1.N
25 CALL SYMC(UL+DLZ,LNGTH(KU)-BOTTOM)*.1+NSTMB,96**1)
30 IF(KU.EQ.KU2)SYMB=4
C DRAW A DOTTED LINE FOR THE CONTINUUM LEVEL
C (IF POSITIVE)
IF(INT(NARG)+L.T.0.)GO TO 20
U=INT(INT(NARG)
L=DX*(TOP+BOTTOM)
DL=L/69.
DO 18 KU=1,35
CALL PLOTC(U,L+3)
18 CALL PLOTC(U,L+DL)
C PLOT THE EXPERIMENTAL POINTS
C IF(KU.EQ.KU2)SYMP=0
IF(LNGTH(KU).LT.BOTTOM .OR. LNGTH(KU).GT.TOP) GO TO 30
U=0.
KSHOT=1.N
DO 25 KSHOT=1.N
25 CALL SYMC(UL+DLZ,LNGTH(KU)-BOTTOM)*.1+NSTMB,96**1)
30 IF(KU.EQ.KU2)SYMB=4
C DRAW AXES
CALL AXISN(O.,O.,NTICY HEIGHT-.1,180.)
CALL AXISN(O.,G..NTICX WIDTH,.1,90.)
C DRAW AXES
CALL PLOTC(U,L,3)
C PLOT THE EXPERIMENTAL POINTS
C (IF POSITIVE)
DO 30 K=1,N
C IF(KU.EQ.KU2)SYMP=0
IF(LNGTH(KU).LT.BOTTOM .OR. LNGTH(KU).GT.TOP) GO TO 30
U=0.
KSHOT=1.N
DO 25 KSHOT=1.N
25 CALL SYMC(UL+DLZ,LNGTH(KU)-BOTTOM)*.1+NSTMB,96**1)
30 IF(KU.EQ.KU2)SYMB=4
C DRAW A DOTTED LINE FOR THE CONTINUUM LEVEL
C (IF POSITIVE)
IF(INT(NARG)+L.T.0.)GO TO 20
U=INT(INT(NARG)
L=DX*(TOP+BOTTOM)
DL=L/69.
DO 18 KU=1,35
CALL PLOTC(U,L+3)
18 CALL PLOTC(U,L+DL)
C PLOT THE EXPERIMENTAL POINTS
C (IF POSITIVE)
DO 30 K=1,N
C IF(KU.EQ.KU2)SYMP=0
IF(LNGTH(KU).LT.BOTTOM .OR. LNGTH(KU).GT.TOP) GO TO 30
U=0.
KSHOT=1.N
DO 25 KSHOT=1.N
25 CALL SYMC(UL+DLZ,LNGTH(KU)-BOTTOM)*.1+NSTMB,96**1)
30 IF(KU.EQ.KU2)SYMB=4
C DRAW AXES
CALL AXISN(O.,O.,NTICY HEIGHT-.1,180.)
CALL AXISN(O.,G..NTICX WIDTH,.1,90.)
C DRAW AXES
CALL PLOTC(U,L,3)
***** THEORY (AXIS) *****

SUBROUTINE AXIS (XX, YY, N Tic, ALNTH, TIC, ANGLE)

NAME***

AXIS

PURPOSE***

TO DRAW ONE AXIS FOR A 2-DIMENSIONAL GRAPH

USAGE***

CALL AXIS (XX, YY, N Tic, ALNTH, TIC, ANGLE)

XX, YY R#1 POSITION OF START OF AXIS (INCHES FROM PAPER ORIGIN)

N Tic R#1 NUMBER OF LINE SEGMENTS (TICKED) TIC MARKS

ALNTH R#1 LENGTH OF AXIS (INCHES)

TIC R#1 LENGTH OF TIC MARKS (INCHES)

TIC<0,0 FOR 0 MARKS ON CLOCKWISE SIDE

TIC>0,0 FOR MARKS ON COUNTERCLOCKWISE SIDE

ANGLE R#1 ANGLE OF AXIS FROM X-AXIS (DEGREES)

A=ALNTH/N Tic

X=XX

Y=YY

CX=COS(0.017453*ANGLE)

CY=SIN(0.017453*ANGLE)

XX=XX+AX

YY=YY+AY

TX=0

TY=TIC

CALL PLOT (XX+TX, YY+TY, 3)

DO 10 I=1, N Tic

CALL PLOT (XX+TX, YY+TY, 2)

XX=XX+AX

YY=YY+AY

10 CALL PLOT (XX+TX, YY+TY, 2)

CALL PLOT (XX+TX, YY+TY, 3)

RETURN

END

*EJECT

ORIG. PAGE 117 OF POOR QUALITY
***** THEORY (PL/C) *****

SUBROUTINE KEYS(ARG1HARG)

NAME...

4USG

PURPOSE...

TO CONVOLVE THE THEORETICAL AND THE INSTRUMENT PROFILES

CALLING SEQUENCE...

CALL NEWS(ARG1HARG)

ARG  R: I  ARRAY OF NONLINEAR PARAMETERS

ARG(1) IS THE ELECTRON DENSITY TIMES 1.E-16.

NARG I  NUMBER OF NONLINEAR PARAMETERS PRESENT.

METHOD...

THE HOLTZMARK FIELD STRENGTH IS CALCULATED AND USED TO FIND

THE AMOUNT OF BROADENING NEEDED IN (S(ALPHA), ALPHA)

SPACE. THIS IS ACCURATE IF THE FINAL ELECTRON DENSITY IS

CLOSE TO THE ORIGINAL ESTIMATE USED HERE. THE GAUSSIAN

HERMITE QUADRATURE FORMULA USED HERE IS EXACT FOR THE

INTEGRAL OF A GAUSSIAN INSTRUMENTAL PROFILE AND A FIFTH ORDER

CURVE FOR THE THEORETICAL PROFILE.

INCLUDE BLANKLIST

DIMENSION ARG(1)

WE USE THE HOLTZMARK FIELD STRENGTH

F0=1.2603*10.4 .RD3E=10*E** (2/3)

F0=1.2603*10.4 .ARG(1)* .RD3E66666666667

WE USE THE ORTHOGONAL FOR THE 3 POINT GAUSSIAN

HERMITE QUADRATURE FORMULA

DELTA( +Wn/F0)=SORT(3/(2*ALOG(2)))

DELTA=1.4716695569/F0

N=NS1

DO 10 KS=2*N

ALPH2(KS+1)=ALPH1(KS)

10 SALPHI(KS+1)=1666666666*

VALUE(ALPH1), SALPHI, IS1*ALPH1(KS) - DELTA(1)

VALUE(ALPH1, SALPH1, IS1 ALPH1(KS) - DELTA(0))

ALPH2(1)=ALPH2(1)

SALPH2(1)=SALPH2(1)

VALUE(ALPH1, SALPH1, IS1, DELTA(0))

ALPH2(1)=0.

RETURN

END

*EXCT
SUBROUTINE NEWT(ARG,NARG)

NAME...

PURPOSE...

TO CALCULATE THE PROFILE IN WAVELENGHT SPACE,knowing
THE ELECTRON DENSITY AND THE PROFILE IN (S,ALPHA),ALPHA)
SPACE

CALLING SEQUENCE...

CALL NEWT (ARG,NARG)

ARG K+1 ARRAY OF NONLINEAR ARGUMENTS.
NARG I+1 NUMBER OF NONLINEAR ARGUMENTS

INCLUDED DUMMY LIST

DIMENSION ARG(3)

WE USE THE HOLTMPK NORMAL FIELD STRENGTH

IF(ARG(1)+.0+.0)GO TO 90

FO=1.2503E-9*(1.16*ARG(1))**.060667

N=N+2

DO 20 KS=2,N

DEL(KS)=FO+ALPH2(KS)

20 CONTINUE

GET

RETURN

PRINT 901,ARG(1)

901 FORMAT (* NEWT: DENSITY OF*,G9.5,*,1.E16 *,*)

STOP

END

*EXPT

ORIGINAL PAGE IS OF POOR QUALITY
SUBROUTINE NEWU(ARGU,NARGU)

INCLUDE DBANK.LIST
INCLUDE GROUP.LIST
DIMENSION ARGUM(4)
A:ARGUM(2)+BASE
DO 15 J=INARGU+1
SU(I,J)=0
DO 25 K=1,NARGU
T=VALUE(TDEL+TSEL,LENGTH(KU)+1)
SUM(KU+1)=SUM(KU+1)+T*T
SUM(1,2)=SUM(1,2)+T*N
SUM(1,3)=SUM(1,3)+T*EXP(KU,KSHOT)
SUM(2,3)=SUM(2,3)+T*EXP(KU,KSHOT)
CONTINUE
SU(1,2)=TOTAL
SAVE ELEMENTS FOR CALCULATION OF VARIANCE-
COVARIA'CE MATRIX
COVAR(3,3)=SUM(1,1)
COVAR(3,4)=SUM(1,2)
COVAR(4,4)=SUM(1,2)
HAVE THIS SYMMETRIC SYSTEM SOLVED
CALL SYMSLV(SUM,COVAR,NARGU+1,NARGU+1,NARGU+1,40)
RETURN
40 PRINT 908
908 FOR4AT(' SINGULAR MATRIX!!')
STOP
END
FUNCTION SIGMA(A,M)

C

PURPOSE...

C

TO FIT THE MEAN SQUARE DEVIATION OF THE DATA FROM THE
VALUES PREDICTED USING THE CURRENT PARAMETERS.

C

INCLUDE BANK.LIST

DIME IDEM ANG(4)

LOGICAL OPT

SIGMA=0.

AZANG(2)+BASE

DO 20 KU=1,2

T=VALUE(DEL*PIEL)+SQA+LENGTH(KU),0

U=SUM(1,3)+T*SUM(2,3)

N=XSHOT(KU)

DO 20 KSHOT=1,N

20 SIGMA=SIGMA+((INTERP(KU,KSHOT)-U)**2

RETURN

END

**EJCT**
THEORY (SYMSLV)

SYMPLTGIC SYMSLV(A,U=N,N,IT=5)
1
NAME...

SYMMETRIC LINEAR EQUATION SOLVER
2
CODE NAME...

SYMSLV
3
PURPOSE...

TO SOLVE A LINEAR SYSTEM AX=B WHEN THE MATRIX A IS
4
SYMMETRIC AND POSITIVE DEFINITE. THE ROUTINE CAN BE
5
CALLED SUCCESSIVELY TO PERFORM THE SOLUTION FOR
6
A NEW RIGHT HAND SIDE WITHOUT DECOMPOSING AGAIN.
7
CALLING SEQUENCE...
8
9
CALL SYMSLV(A\ B, N, N, IT=5)
10

ARGUMENTS ON ENTRY:

A MATRIX OF COEFFICIENTS. SINCE IT IS SYMMETRIC,
11
ONLY ELEMENTS HFFED ARE A(I,J), I.LE.I.LE.J.LE.N.
12
B ARRAY OF ELEMENTS FROM RIGHT HAND SIDE
13
N DIMENSION OF MATRIX AND A.
14
N1 MAXIMUM NUMBER OF ROWS IN A (FIRST DIMENSION)
15
IT SWITCH... IT=1 IF MATRIX A WAS DECOMPOSED ON A
16
PREVIOUS CALL TO SYMSLV, AND ONLY THE ARRAY B
17
IS DIFFERENT THIS TIME. IT=1 IF A IS NEW.
18
$50 CONTROL WILL BE PASSED TO THIS STATEMENT IF
19
A PIVOT ELEMENT IS FOUND OF ABSOLUTE VALUE
20
LESS THAN 1.E-10.
21

ARGUMENTS ON RETURN:

A ORIGINAL MATRIX IS DESTROYED. LOWER TRIANGLE HOLDS
22
LOWER TRIANGLE OF MATRIX L. (DIAGONAL ELEMENTS OF L
23
ARE 1.S.) DIAGONAL ELEMENTS HOLD MATRIX D.
24
B SOLUTION ARRAY X.
25

METHOD...

SYMMETRIC FACTORIZATION IS USED TO FIND A LOWER
26
TRIANGULAR MATRIX L AND A DIAGONAL MATRIX D SUCH
27
THAT A=LDO WHERE U IS L TRANSPOSED. THE UNKNOWN
28
VECTOR IS CALCULATED BY BACK SOLVING THESE TRIANGULAR
29
SYSTEMS: UZ=B, DY=Z, LX=Y.
30
DIMENSION B(5),A(25).
31
IF(N.GT.1)GO TO 10
32
B(1)=L(1)/A(1)
33
RETURN
34
10 IF(IT.EQ.1)GO TO 28
35
DO 25 K=1,N-1
36
IF(ABS(A(K+K-1)) .LT. 1.E-10)RETURN 6
37
DO 25 J=K+1,N
38

25 CONTINUE
***** THEORY (GTHSYL) *****

57     S=A(K+M+J-1)/A(K)+J*K+i
60     DO 20 J=1,N
71     DO 30 J=2,N
72     30 DO 39 J=1,N-1
73     39 B(J)=B(J)-S*(J+1:N)@N)@B(J)
80     DO 90 J=1,N
90     90 DO 89 J=1,N-1
89     89 B(J)=B(J)+S*(J+1:N)@N)*B(J)
92     RETURN
93     END

*END

ORIGINAL PAGE IS OF POOR QUALITY
THEORY (VALUF)

FUNCTION VALUE(X,Y,N,XP,,N)

NAME: VALUE

PURPOSE: TO INTERPOLATE IN A TABLE TO FIND INTENSITIES FROM THE THEORETICAL LINE PROFILE.

CALLING SEQUENCE:

CALL VALUE(WAVF,INT,N,WANT,P)

WAVE R INT N WANT P VALUE

ARRAY OF WAVELENGTHS (DISPLACEMENTS FROM LINE CENTER)

ARRAY OF CORRESPONDING LINE INTENSITIES

NUMBER OF ENTRIES IN WAVE OR INT

ARRAY OF WAVELENGTH AT WHICH INTENSITY IS DESIRED

A WORK ARRAY OF LENGTH N. P(I) IS USED TO STORE A POINTER BETWEEN CALLS. SO EACH SEARCH OF WAVE REGIONS WHERE THE PRECEDING SEARCH ENDED.

METHOD: BEYOND THE END OF THE TABLE, A 9/2 POWER LAW IS USED TO EXTRAPOLATE. WITHIN THE TABLE, AKIKER'S PROCEDURE IS APPLIED USING 4 POINTS. SINCE AN EVEN NUMBER OF POINTS IS USED, THE INTERPOLATING FUNCTION IS CONTINUOUS.

DIMENSION X(N),Y(N),P(4)

EQUIVALENCE(SAVE,J)

IF(XBAR.GE.X(N))GO TO 90

RETRIEVE POINTER FROM LAST CALL

SAVE=P(1)

ENSURE 1 .LE. J .LE. N

IF(XBAR-X(J))4,80,20

CONTINUE

IF(XBAR-X(J))10,80,22

CONTINUE

SEARCH DOWN

IF(J.LE.1)GO TO 50

JSTART=J

DO 12 J=JSTART+2,-1

IF(XBAR-X(J))12=75;40

CONTINUE

J=1

GO TO 50

SEARCH UP

IF(J.GE.N)GO TO 30

JSTART=J+1

DO 22 J=JSTART+1

IF(XBAR-X(J))140;80;22

CONTINUE

J=N-3

GO TO 50
***** THEORY (VALUE) *****

**SAVE THIS POINTER**

**SET J TO POINT TO FIRST OF THE 4 POINTS**

**IN Y NEAREST XBAR**

**APPLY ATHERN'S PROCEDURE USING 4 POINTS**

**THE GROUP OF STATEMENTS TO FOLLOW IS EQUIVALENT TO:**

DO 60 1=2 TO J-1
60 P(I)=Y(J-1)

DO 60 L=2 TO J
60 P(I)=(P(L-1)*(X(J+L-1)-XBAR)-P(I)*(X(J+L-2)-XBAR))/
- ((X(J+1-I)-XBAR)(X(J+L-1)-XBAR))

**DO CONTINUE**

...**BUT (WITHOUT LOOP CONTROL) WILL EXECUTE FASTER**

**SAVING THE POINTER IN THE WORK ARRAY**

**RETURN**

**RETURN**

**RETURN**
REFERENCES


26. J. W. Strutt (Baron Rayleigh), Phil. Mag. 27, 298 (1889).


42. H. R. Griem, private communication.


