GA-8705

# FINAL REPORT

for

# COLLISIONS OF ELECTRONS AND IONS WITH HYDROGEN ATOMS

(8 May 1967 - 7 May 1968)

Contract No.: NAS 5-11025

Prepared by
Gulf General Atomic Incorporated
P.O. Box 608, San Diego, California 92112

for

Goddard Space Flight Center
Greenbelt, Maryland

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## ABSTRACT

A study of 2p excitation of the hydrogen atom under electron impact is reported. The major finds have been the resonance structure just above the threshold of excitation, which was not predicted, and just below the threshold of n = 3, which was predicted but which for higher angular momentum states does not agree with theory. Resonance structure above n + 3 has also been observed.

Dissociative excitation of $H_2$ and $D_2$ has been studied under high electron energy resolution. Several new dissociation channels have been identified. Gaseous filtering techniques to be applied to radiations in the vacuum ultraviolet were studied. Some of the computer codes used on this program are given in the report, along with abstracts and papers published this year.

CONTENTS



FIGURES

TABLE

# 1. INTRODUCTION

During the past year, primary attention has been focused upon the collision of highly resolved electrons with hydrogen atoms leading to the excitation of the lowest radiative state of the atom, i.e.,

$$e + H(1s) = H(2p) + e \quad .$$

As in the case of elastic scattering of electrons from hydrogen atoms, inelastic scattering, particularly in the vicinity of the various levels of the hydrogen atom, is dominated by the formation of the temporary compound negative ion states.

In Section 3 of this report, the resonances found in the 2p channel immediately above the excitation threshold are discussed; in Section 4, those below and above the n = 3 level of the hydrogen atom are considered. In Section 5, a comparison is made between the measured cross section in the vicinity of threshold and the best calculated values.

Complementing the study of electrons colliding with the hydrogen atom, a study has been made of the collision of electrons with the hydrogen molecule and the subsequent dissociative excitation of the 2p state of the hydrogen atom,

$$e + H_2 = H(2p) + H(1s) + e$$

in competition with

$$e + H_2 = H(2p) + H^- \quad .$$

The contribution to 2p excitation from the second reaction is small. The measurements made on $H_2$ are unfortunately complicated by ultraviolet radiation other than Lyman-alpha which passes through the few narrow windows in the $O_2$ filter. In Section 6, the results of a short study of gaseous and chemical filters are discussed; in Section 7, the results of dissociative excitation are reviewed.

Since the primary purpose of the program is to test theory and to relate the results with the theory, we have been conducting under NASA's support a small theoretical program. This program is discussed in Section 8.

Because of the extreme complexity of the 2p excitation problem, we have developed a number of computer codes to process and analyze the data in next year's program. In Section 9 these codes are discussed and are thus made generally available to the scientific community. Finally, Section 10 presents a discussion of other activities that have complemented the program.

Abstracts of papers presented at scientific meetings appear in Appendix I, and articles that resulted from studies made on this program are included as Appendix II.

## 2. NEW INSTRUMENTATION

The apparatus used this year is essentially that used last year except for minor changes in electronics and the addition of a photo detector on a rotating table. The photo detector was designed to detect Lyman-alpha radiation. During this period two types of photon counter were used. The first was the iodine-filled Geiger counters developed some years ago in this laboratory. This was replaced by an Electromechanical Research multiplier photo tube with lithium fluoride optics. It is an 18-stage silver magnesium dynode multiplier with a potassium bromide photocathode. The geometry chosen had a side window.

The spectral sensitivity of the tube extended from 1050 Å to 1500 Å with very high sensitivity at the Lyman-alpha level (1216 Å). This new photo tube has the necessary characteristic that long wavelengths are amply rejected. The photo tube was chosen to replace the iodine-filled Geiger counter for two reasons. First, estimates indicated that the photo tube would be from a factor of 3 to 10 more sensitive than the Geiger counter. Second, since the experiments required extensive counting times, extreme reliability of all parts was necessary. It was felt that the photo tube, which has essentially infinite lifetime, would be a sensible substitute for the Geiger counter, which is unpredictable in its operating characteristics and comparatively short lived.

Unfortunately, the expectations for the sensitivity of this tube have not been met. At the very most, sensitivity has been increased by a factor of 2. However, since the time of its installation six months ago, the photo tube has required no service even though it has been in continuous operation for most of this time.

Between the photo detector and the interaction volume defined by the electron and hydrogen atom beams, a 1-cm-long cell with lithium fluoride windows is placed and is filled with molecular oxygen. It is a strange quirk of nature that in the absorption spectrum of molecular oxygen, one of seven very narrow windows is centered around Lyman-alpha, i. e., at 1216 Å. For the chemical (gaseous) filter to pass Lyman-alpha, the oxygen must be dry. If any moisture is present, the transmission of the cell can be greatly reduced. Consequently, dried oxygen is continuously flowed through the cell.

The experimental demands associated with the study of 2p excitation of atomic hydrogen have been excessive. The experiments have required the complete stability of the electronics, the electron beam, the hydrogen atom beam, etc., over periods well in excess of 24 hr to collect a significant number of data. In many experiments, data have been taken in 0.015-V intervals with from 60 to 100 points per cycle. For each cycle, then, the total interval is 0.9 eV for 60 data points and 1.5 eV for 100 data points. The normal counting time per data point is 1 min. If there are 60 points per cycle, the time for one cycle is 1 hr. It is interesting to compare the results that can be obtained from one cycle with those that can be obtained when a number of cycles are summed together. An example (Run 39C) is given in Figs. 1 and 2. Figure 1 shows one of 35 cycles, while in Fig. 2 all 35 cycles have been summed. In the single cycle, no feature is recognizable. In the composite Fig. 2, the 2p excitation threshold is clearly defined and the resonance near the threshold can be seen. The randomness observed below threshold gives some idea of the fluctuation of the background.

At the peak of the resonance, Fig. 2 shows approximately 300 counts for the integrated signal. One standard deviation for the (signal plus background) and background combined is approximately ±30 counts. The resonance peak, as shown in Fig. 2 and in many of the earlier runs, was only slightly more than twice this standard deviation.

To define the first resonance above the 2p excitation threshold and to determine whether or not there are subsequent resonances, it was necessary to conduct an experiment that ran for 109 cycles. In this instance, there were 40 points per cycle. The time required for continuous running was in excess of 70 hr.

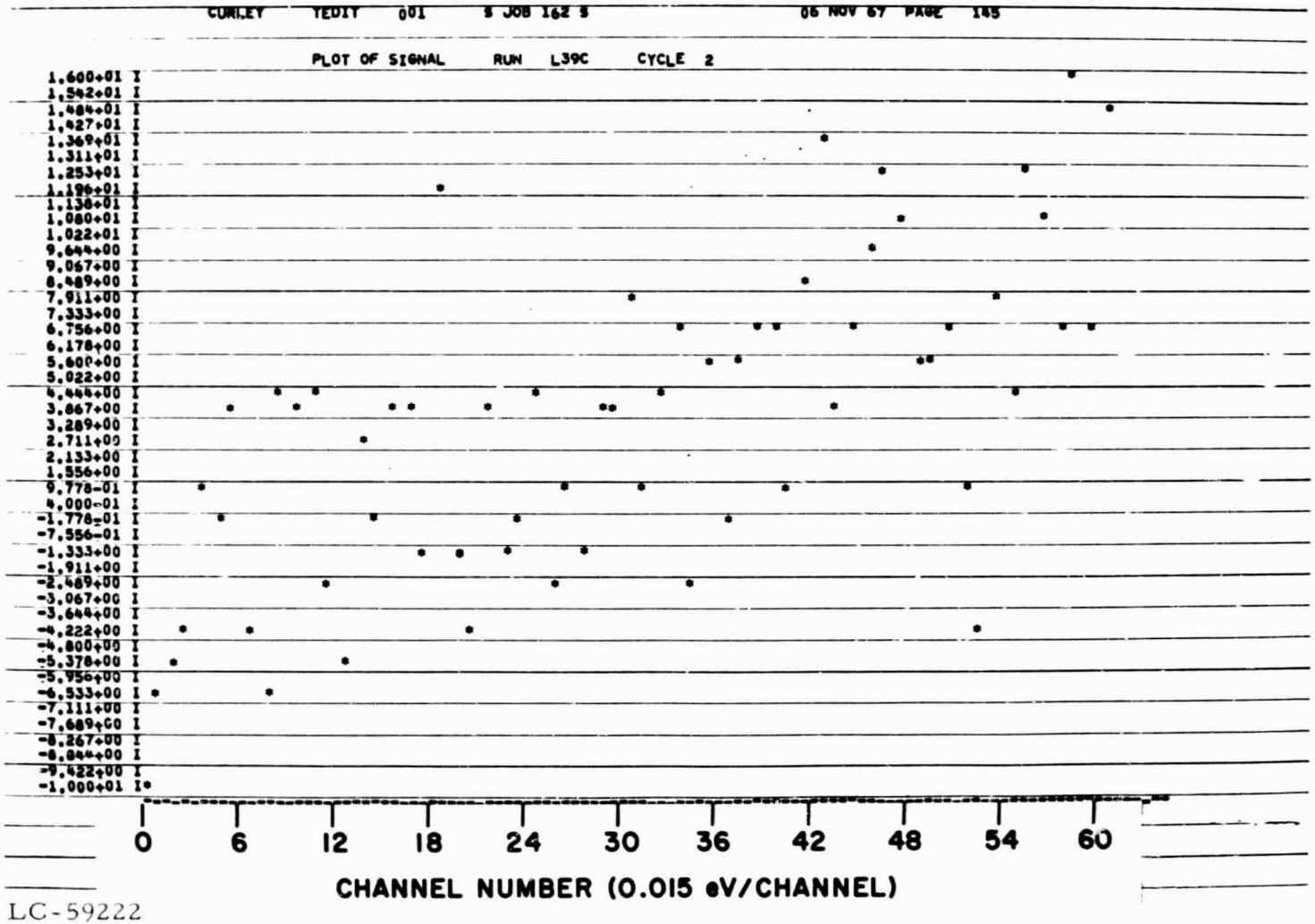


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Fig. 1. One cycle of 35 from run 39C showing the threshold region for 2p excitation. In the single cycle no feature is recognizable.

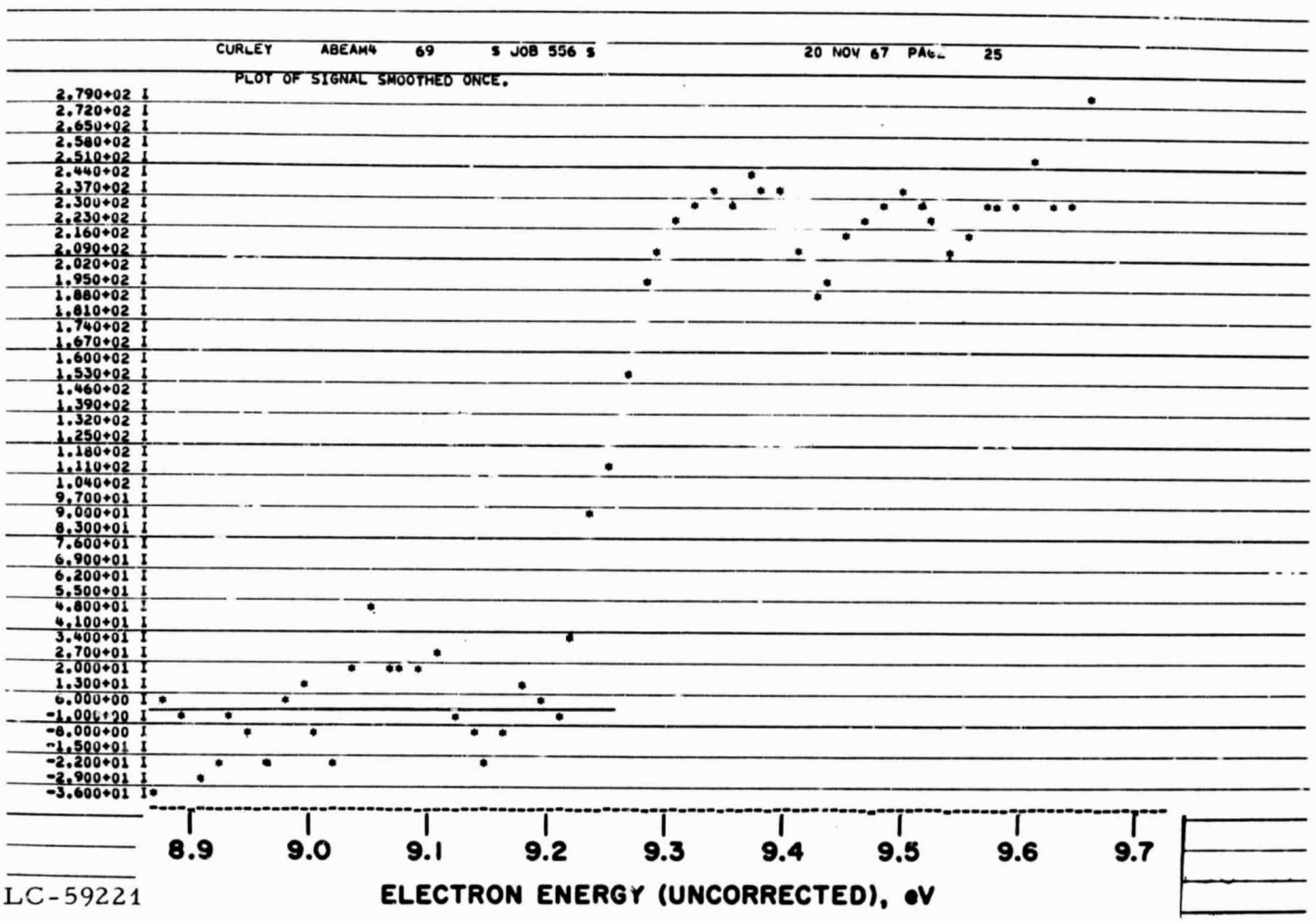


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Fig. 2. The summation of 35 cycles where the sharp rise at the excitation threshold and a hint of the resonance structure just above threshold are quite evident

## 3. THE 2p EXCITATION THRESHOLD

In this section, we discuss the excitation of H(2p) from threshold to 0.6 eV above threshold. The collision region is shown schematically in Fig. 3. A modulated rectangular beam of hydrogen atoms nearly 90% pure is crossed with a rectangular beam of electrons with an energy distribution that ranges from 0.06 eV to 0.18 eV. Electrons from a source 127° electrostatic electron energy analyzer enter a magnetic and electric field free region, cross the modulated hydrogen atom beam from below, and pass into a collector in which a crossed electric field can be applied to collect all the electrons. When this crossed field is removed, the electrons can pass through the collector to a second electrostatic energy analyzer, where the energy distribution of the electrons is measured.

Photons from the interaction of the two beams were normally detected at an angle of 54.5° with respect to the direction of the bombarding electrons. At this angle the measured signal was proportional to the total 2p excitation cross section.[1] Ions from the interaction region were accelerated along the atomic beam axis into a Paul mass filter. As in previous experiments at this laboratory, the linear extrapolation of the ionization efficiency curve to its energy axis was used as a calibration for the electron energy scale. The data were recorded automatically over many hours, as described in Section 2. The system can be programmed to step through a prescribed energy interval. All data were collected digitally; i.e., for each energy interval, the signal plus background (S+N), the background (N), and the electron current were recorded on punched tape to be processed later by the computer. Every 8 to 12 hr, the excitation process was interrupted and an ionization efficiency curve for atomic hydrogen was taken to help fix the electron energy scale for excitation. Over more than 100 hr, in many instances the reproducibility of the onset of the ionization efficiency curves was within ±0.015 eV.

In Fig. 4, the total cross section measurements near threshold are compared with theory[2] and with the previously reported results of Chamberlain et al.[3] This comparison is made primarily to show the difference between the resolutions of the two experiments and the width of the structure that one is looking for compared with what has been observed experimentally. In the left-hand portion of Fig. 5, theoretical results are compared with the theoretical predictions wherein the energy

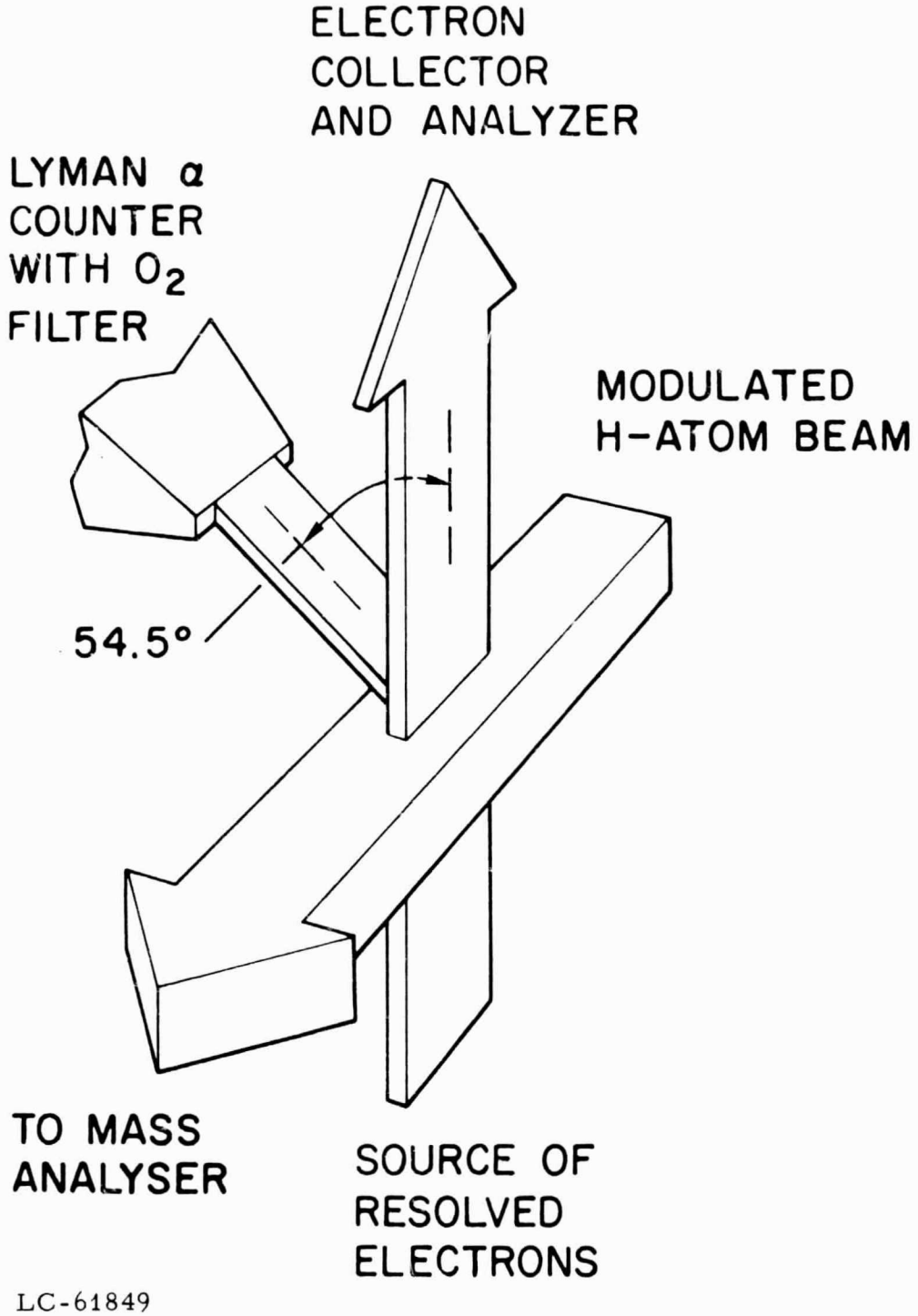



Fig. 3. A sketch of the electron hydrogen atom collision region showing roughly the geometry used in the experiment

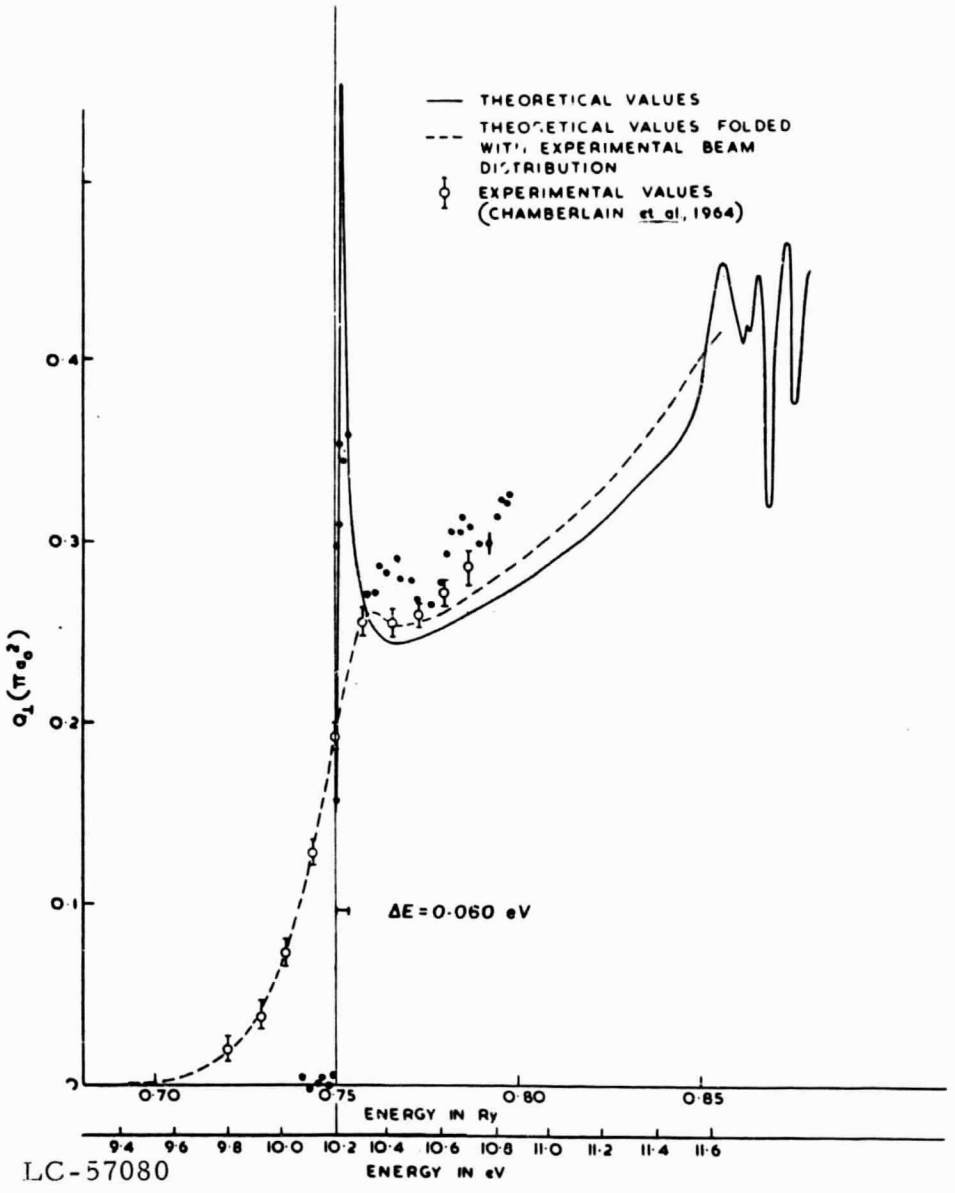



Fig. 4. The solid curve is the 2p excitation cross section calculated by Burke et al. for the cross section observed at 90° to the direction of the bombarding electrons. The open circles are the low resolution data (0.35 eV) of Chamberlain et al. for the Lyman-alpha measured at 90° to the electron path. The experimental value has been normalized to the theoretical. The data represented by the closed circles are for a resolution of 0.07 eV. They too have been normalized to the theoretical cross section but are proportional to the total cross section rather than that at 90°.

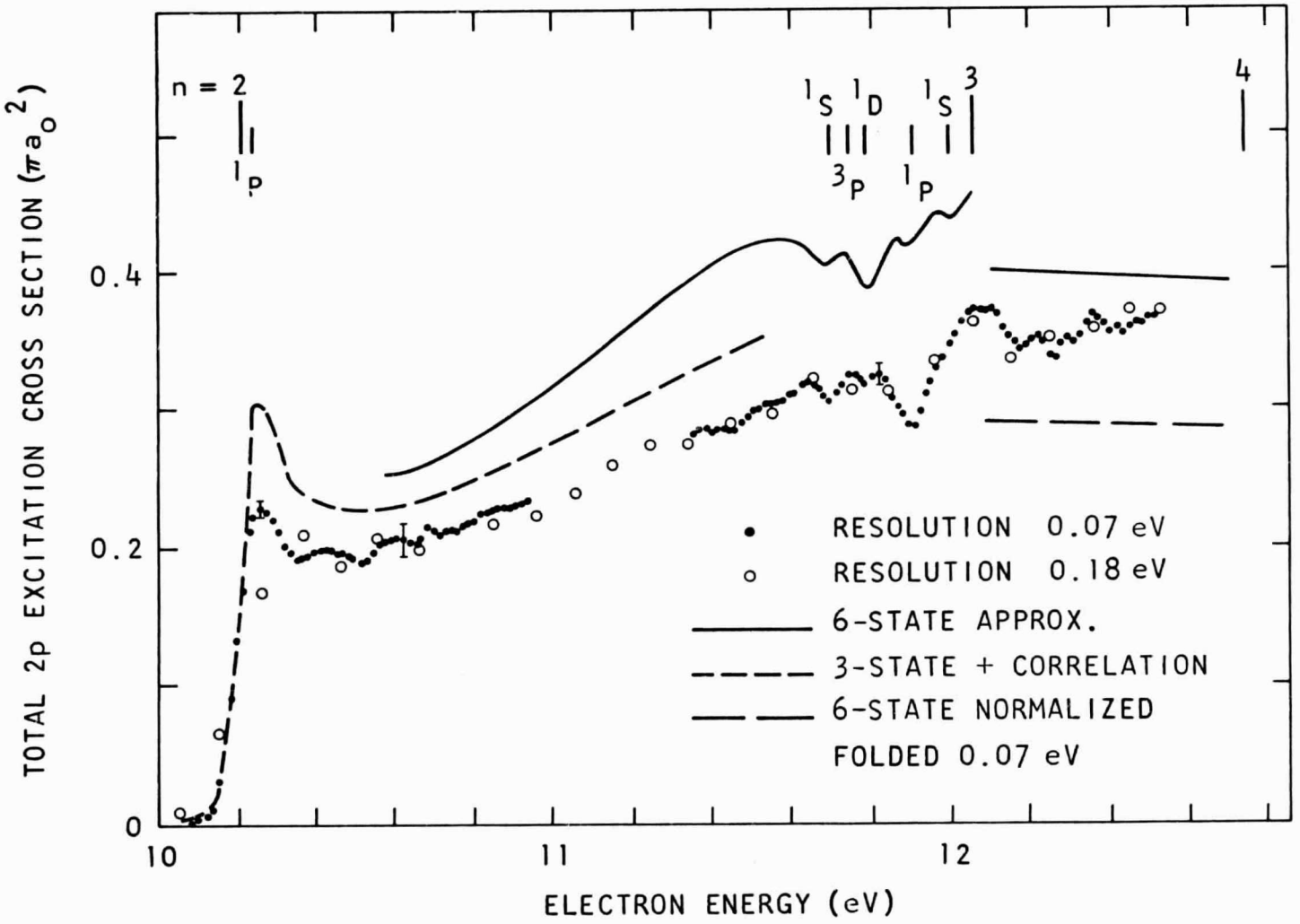



Fig. 5. Theoretical and experimental values for the total excitation cross section in the vicinity of threshold. From threshold to 10.5 eV the statistical uncertainty is approximately ±1%. Between 11.60 and 12.20 the uncertainty is less than ±2%. For the rest of the 0.07-eV resolution data it is ~3%.

distribution, approximately 0.07 eV, has been folded into the theoretical curve. As can be seen, the agreement between the measured and predicted shapes of the first resonance is good. It follows, then, that the excitation cross section does consist of a sharp rise, as predicted by Damburg and Gailitis,[4] from a close-coupling approximation calculation that includes the three lowest hydrogen atom states, 1s, 2s, and 2p. It is also clear from our measurements that the sharp resonance predicted by Taylor and Burke,[5] who also used a close-coupling approximation, does really exist within 0.03 eV of threshold. Burke and his associates have shown that the total flux of this resonance is in the $^1P$ channel of the $H^-$ compound state. This resonance unfortunately was not recognizable in the previous calculations of Damburg and Gailitis because of the coarseness of the energy grid used by them.

In the experimental results immediately following the first resonance, there appear to be at least two other broad resonance structures. Although these structures have been recognized from our earliest measurements, it was only recently that the statistics were good enough to permit us to say definitely that they exist. It was also necessary to make certain that these small structures were not due to the excitation of some countable ultraviolet from the collision of electrons with the residual $H_2$ in the system. Table 1 lists the positions of the most promient structures; however, one must remember that these positions may not correspond exactly to the positions of the resonances themselves, but rather to the resonances with the electron energy distribution folded into them.

The use of the finite number of terms in the close-coupling expansion used to describe even these lowest states may be subject to some question since it is not clear how quickly the expansion converges. In the case of the elastic scattering resonances below the first inelastic threshold n = 2, there is every indication that the convergence is rapid. However, it is not yet clear that the $^1P$ "shape" resonance described by the three-state approximation above  = 2 is not better described by an expansion that includes the first six or more states of the hydrogen atom. Unfortunately, Burke et al.[2] have carried out their six-state approximation calculations only from just below the n = 3 level down to within 0.2 eV of the 2p excitation threshold. Over the range where the three- and six-state approximations overlap, i.e., in the region from 0.2 to 1.0 eV above the 2p threshold, the six-state calculation gives a cross section value approximately 8% lower than that given by the three-state approximation.

Another calculation reported by Taylor and Burke[5] has been carried out using the close-cupling approximation that includes the first three states of the hydrogen atom and potential terms that describe the electron-electron interaction (correlation) as a power series of terms involving $r_{12}$,

the distance between the two electrons. Over the same energy range as taken above, the later calculation gives a cross section value that is approximately 20% below that given by the three-state approximation. Near threshold, the correlation terms have now shifted the calculated resonance closer to the threshold and have considerably reduced its width. This is in keeping with the experimental finding. The need for more work on the theory has recently been recognized by Damburg and Geltman, [6] who indicate that another possible source of incompleteness results from the lack of the inclusion of polarization terms of order $\alpha/r^4$. In the case of 2s excitation, the inclusion of polarization has had a marked effect on the calculated cross section.

TABLE 1

STRUCTURE IN 2p EXCITATION CURVE

| Energy | Description of Structure | Comments |
|---|---|---|
| 10.20 ± 0.02 | Steep slope | Onset |
| 10.29 ± 0.02 | First max | Predicted $^1P$ "shape" resonance |
| 10.45 ± 0.03 | Second max | |
| 10.65 ± 0.03 | Third max | |
| 11.65 ± 0.03 | Small min | Predicted $^1S$ resonance |
| 11.77 ± 0.02 | Possible min | Predicted $^1D$ resonance |
| 11.89 ± 0.02 | Large min | Predicted $^1P$ resonance |
| 12.06 ± 0.04 | Broad max | "Shape" resonance at n = 3 threshold |
| 12.16 ± 0.05 | Min | |
| 12.23 ± 0.05 | Small max | |
| 12.35 ± 0.05 | Small max | |

## 4. THE 2p EXCITATION IN THE VICINITY OF n = 3

Figure 5 shows details of the experimental cross section from 11.35 eV to 12.55 eV. This region overlaps the n = 3 threshold. Bridging the two threshold regions are low resolution measurements. Just below the n = 3 threshold can be seen several recognizable resonances, the most predominant of which appears near 11.88 eV. A smaller resonance appears in the vicinity of 11.65 eV. Also shown in the figure is the calculation for the six-state approximation showing a number of resonances. Folded into the calculated cross section is the experimental energy distribution, which is approximately 0.07 eV. The agreement between theory[2] and experiment is not considered good for the $^1P$ resonance, while for the $^1S$ resonances the agreement is thought to be quite satisfactory.

At and above the threshold of n = 3 can be seen a prominent bump, which is most likely associated with a "shape" resonance just above the n = 3 threshold. Part of the flux for this resonance appears directly in the 2p channel. Another portion, most likely the largest part, arrives through cascade from the 3s and 3d states of the atom. The positions of the resonance structure below and above the n = 3 level are included in Table 1.

## 5. TOTAL CROSS SECTION MEASUREMENTS

Since it is impossible to measure the cross section absolutely, we have determined it from a normalization to the Borne approximation at energies in excess of 200 eV. Although this procedure is not entirely satisfactory, at present there is no simple method available for making an absolute determination. Data have been taken between the 2p excitation threshold and 200 eV; the most precise data, however, have been taken below 60 eV. In fact, continuous data have been taken every 0.1 V from 60 eV until threshold. We have found the most precise way to determine our cross section is to normalize our data to those of Long, Cox, and Smith, who in turn have normalized theirs to the Born approximation. The relative accuracy of their data is ±2%.

Although we have not been able to assign to our data relative accuracies as small as this, we have compared our data with those of Long, Cox, and Smith (see Fig. 6). The cross sections defined by the two sets of data points are indistinguishable. It is interesting to note in our data that the finite excitation threshold is recognizable just above 10.2 eV, even though the resolution in this experiment is only 0.18 eV. Also, one can see a hint of the resonance structure in the vicinity of n = 3 and in the continuously taken data below n = 4.

To obtain an accurate estimate of the cross section in the threshold region, the high resolution data were subsequently normalized to the lowest resolution data, thus fixing the cross section scale. The values of the cross section given in Fig. 4 were fixed in this way. It is interesting to note that the cross section thus obtained is only 80% of the lowest cross section predicted. The approximation used to arrive at the cross section closest to the experimental value is the three-state close-coupling approximation, which includes 20 electron-electron correlation terms.

Quite recently, Fite et al.[8] have determined that the Lyman-alpha radiation emitted by hydrogen 2s atoms in a weak electric field is polarized. Consequently, all earlier measurements or estimates of the 2s excitation cross section are in error since no allowance was made for this polarization. Once the cross sections have been corrected for the polarization, at the cross section maximum, which is in the vicinity of n = 3, the value obtained is only 80% of the lowest predicted cross section resulting from the six-state close-coupling approximation.

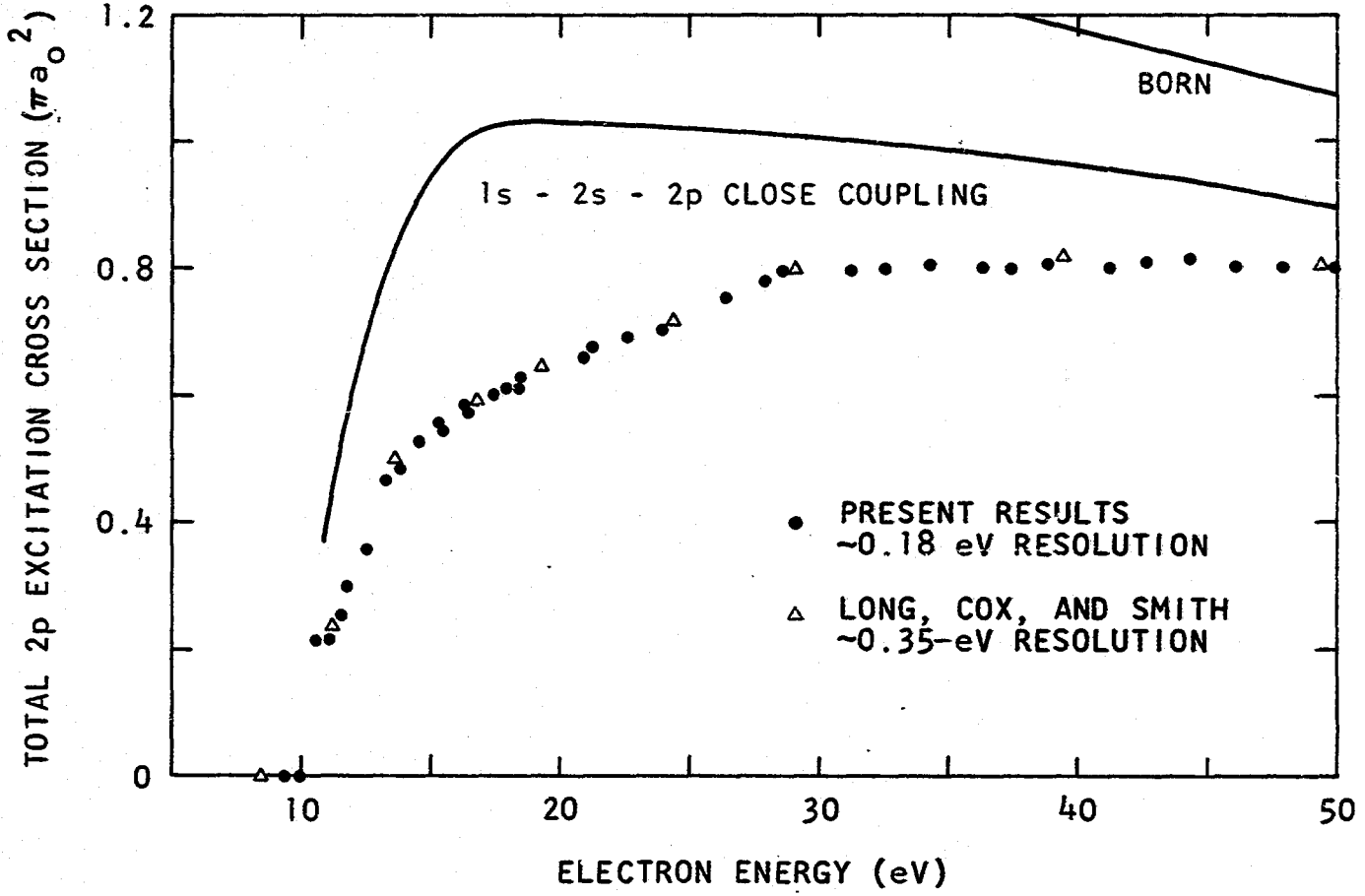



Fig. 6. Comparison of our low resolution results with those of Long, Cox, and Smith to which our results are normalized

It is an informative exercise to estimate the size of the combined excitation cross section for the 3s and 3d states of atomic hydrogen. These data are reflected in the total cross section measurements for the production of the Lyman-alpha radiation since the 3s and 3d cross sections can only couple with the ground state by passing through the 2p state. Although our total excitation cross section for the 2p state does not agree in absolute magnitude with that predicted by Burke et al., it is quite obvious that below the n = 3 level the general shape of the measured and calculated cross sections is the same. Consequently, there is some justification in normalizing the magnitude of the calculated cross section to that of the measured cross section in the region just above the n = 2 level. Having done this, we observe that the calculated portion of the cross section for the 2p state above n = 3 is considerably lower than the total measured cross section (Fig. 5, broken line above n = 3). To a first and perhaps crude approximation, the difference between the measured and normalized theoretical curves can be said to be due to cascade. This difference is shown in Fig. 7. No attempt has been made to include any contribution for the shape resonance above n = 3 in the calculations or to allow for the addition of states above n = 4 in the theory.

It is now possible to compare this difference with the predicted cross sections of Burke et al. As shown in Fig. 7, the agreement between experiment and theory is satisfactory. In fact, even with this crude approximation in which no attempt has been made to account for polarization or other factors, as in the case of 2p excitation, the value of the estimated cross section again lies slightly below that of the predicted cross section. This result is not at all in agreement with the recently published data of Kleinpoppin and Krase[9] for Balmer-alpha excitation. Since our result depends upon a normalizing of the six-state approximation to the results below n = 3, we hesitate to say their result is in error. Furthermore, it is not clear that the six-state approximation necessarily gives an accurate description of the region above n = 3, although it seems reasonable that it is not in error by much.

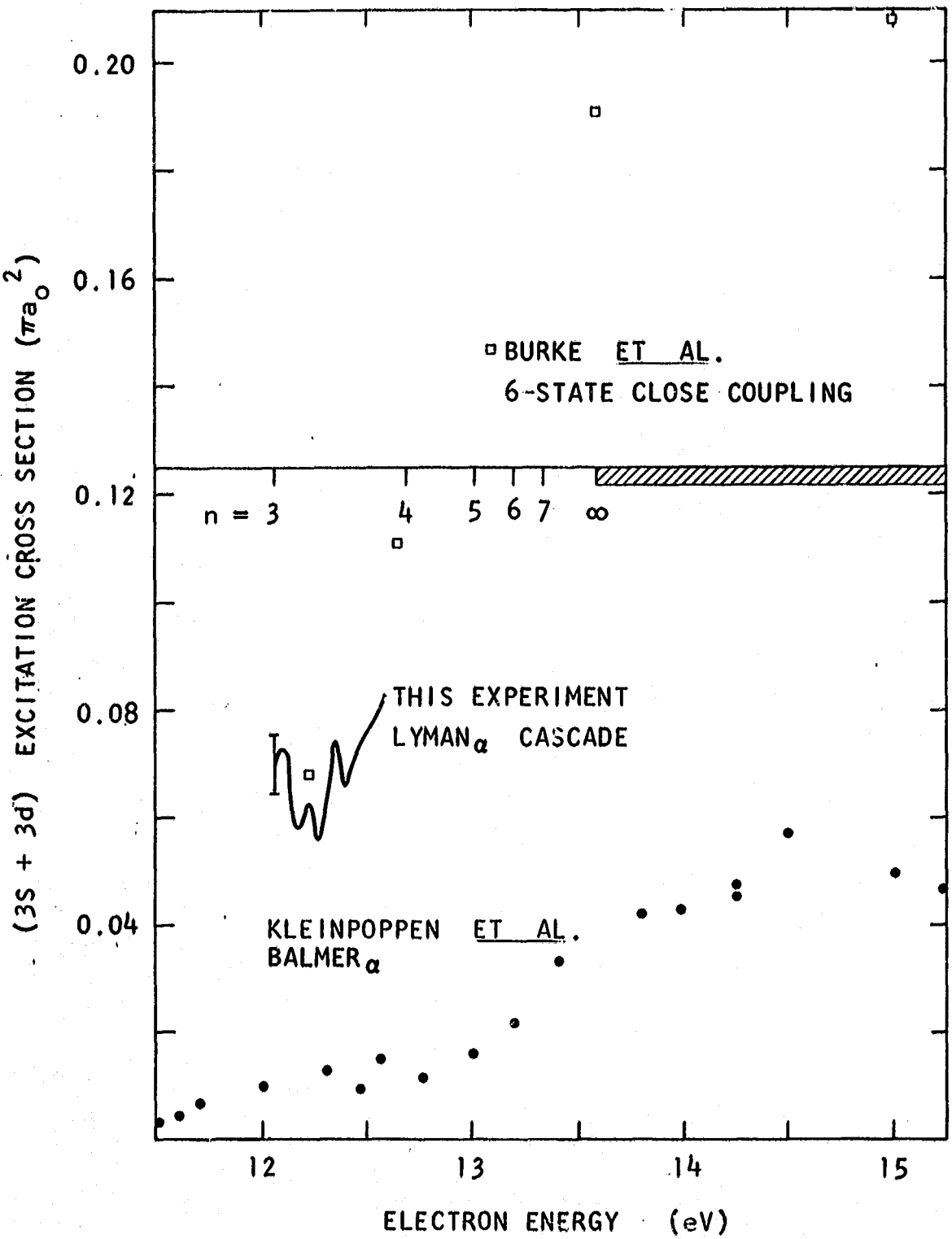



Fig. 7. A cross section for the excitation of the sum of the 3s and 3d states of atomic hydrogen. Shown for comparison are the theoretical value of Burke, Ormonde, and Whitaker and the recent experimental results of Kleinpoppin et al.

## 6. GASEOUS FILTERS

One of the most important problems associated with the study of the excitation of atomic hydrogen is the unequivocal detection of Lyman-alpha (1216 Å). Provided a large enough signal is available from the experiment, one can use a vacuum ultraviolet spectrometer. However, in experiments such as those performed in this laboratory where the number of photons available is very small, it becomes absolutely necessary to have the largest possible collection efficiency and reasonably large angle of acceptance. It has long been recognized that the Geiger counter, filled with either nitric oxide or iodine and with lithium fluoride optics, could be used to detect vacuum ultraviolet radiation in the vicinity of Lyman-alpha. However, to ensure the unequivocal detection of the Lyman-alpha and particularly to eliminate the molecular radiation normally associated with the bombardment of residual $H_2$ in the experiment, it was necessary to find a filter that would preferentially pass the 1216 Å radiation.

It was observed by Watanabe[10] and others that in the absorption spectrum of $O_2$ in the vacuum ultraviolet and in the vicinity of 10 eV there are seven very deep transmission windows, one of which is centered at the Lyman-alpha. It has been the repeated observation in our laboratory that in the study of the excitation of atomic hydrogen to the n = 2 level, the combination of the chemical filter filled with oxygen and either a Geiger counter or a photomultiplier has been an effective detector of Lyman-alpha. However, in the study of the dissociative excitation of $H_2$, either by proton or electron impact, it has been recognized that there is a large contribution of molecular radiation, which passes either through the other windows or through the optically thick portion of the chemical filter.

To effectively study the dissociative excitation process it is therefore necessary to eliminate this background radiation. To do this, a series of experiments was carried out in which different gases were used as the optical filter. In Fig. 8 we show a schematic diagram of our experiment. In all cases the gases used in the chemical filter flowed through the filter continuously. However, in the case of $CO_2$ the rate of flow was much slower than in the cases of nitrogen, helium, and oxygen, which were virtually the same. The pressure in all filters was slightly in excess of 1 atm.

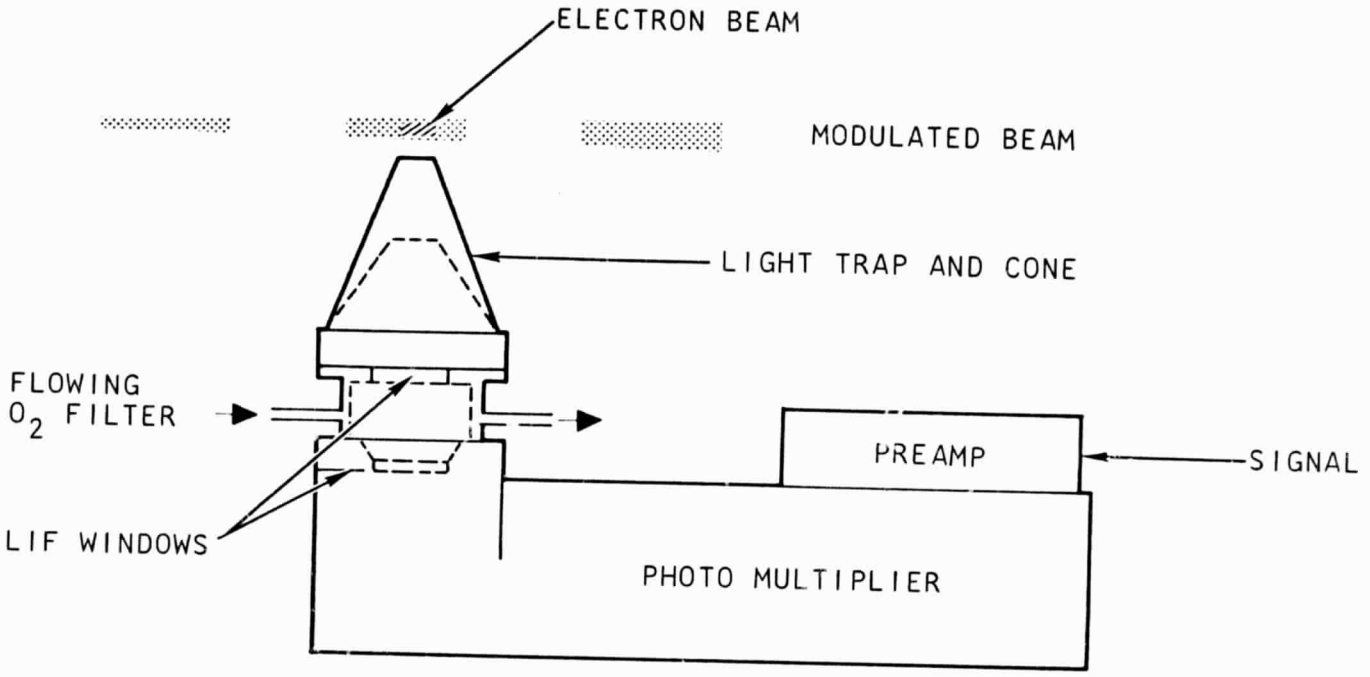



Fig. 8. A schematic diagram of the photodetector and chemical filter used in these experiments

In Fig. 9 we show the relative number of photons reaching the counter as a function of electron energy when electrons bombard $H_2$. Four different gases have been used in the chemical filter. The electron energy for these experiments ranges from approximately 10 to 20 eV, an interval which embraces the onset of the molecular radiation at approximately 10.3 eV and the onset of dissociative excitation in the vicinity of 14.7 eV. Figure 9 shows the results when the $O_2$ filter was used. The onset of the molecular radiation is clearly visible at 10.3 eV, as is the onset of the dissociative excitation of the hydrogen atom in the 2p state near 14.7 eV. From this curve alone we can judge that, once we have moved a few electron volts from the threshold of dissociative excitation, the molecular contribution to the total curve is in the vicinity of 20%. Near threshold for dissociative excitation, of course, the molecular contribution is proportionately larger. Looking at Fig. 9, one can see virtually no difference in the magnitude and shape of the curves for He and $N_2$ (b and c, respectively), verifying what we already know, i.e., that both He and $N_2$ are transparent in this optical region.

Now that we recognize in curve (a) the onset of the dissociative excitation, we can use curves (b) and (c) to estimate the relative contribution of Lyman-alpha and other molecular radiation as seen by the counter. A reasonable extension of the curve, from below the dissociative excitation threshold to above, gives us this information. Above approximately 16 eV we estimate that the radiation from dissociative excitation is in the vicinity of 20% of the total radiation. This estimate, of course, is approximate, but it is reasonable. In curve (d) the complicated absorption spectrum of $CO_2$ is seen reflected in the structure of the curve.

To generate Fig. 10, the helium curve has been normalized to the $O_2$ curve in the vicinity below 14 eV and the helium curve has been subtracted from the $O_2$ curve in this region. The residual signal is shown in Fig. 10. The fine structure below 14.7 eV appears to be real for it is present in the curves when either helium or nitrogen is subtracted from the oxygen data. In both cases there is a sharp onset in the vicinity of the dissociative excitation threshold. It is interesting to note that above 16 eV, structure is quite pronounced in the curve.

It must be realized that by subtracting the helium (or nitrogen) data from the $O_2$ data, we have eliminated part of the dissociative excitation signal in the vicinity above the dissociative excitation threshold. However, this is small (20% of 20%), approximately 4% of the total signal. From this study it is clear that the estimates of the total cross section made earlier by Fite and Brackmann[1] are high by approximately 20%.

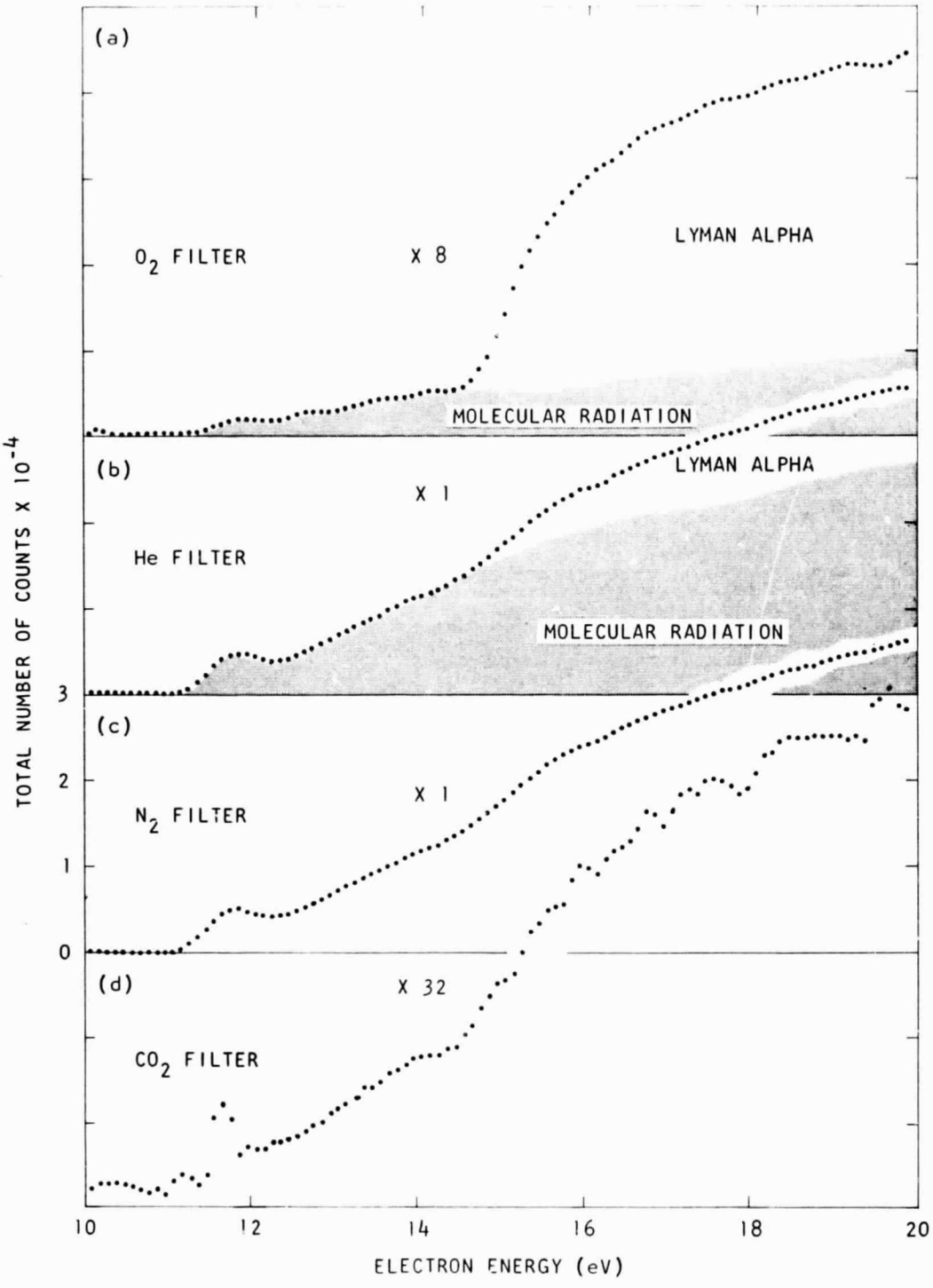



Fig. 9. Relative excitation curves obtained with four different chemical filters: (a) molecular oxygen; (b) dry atomic helium; (c) dry molecular nitrogen; and (d) dry $CO_2$. The pressure in the $CO_2$ filter is slightly higher than in the other filters

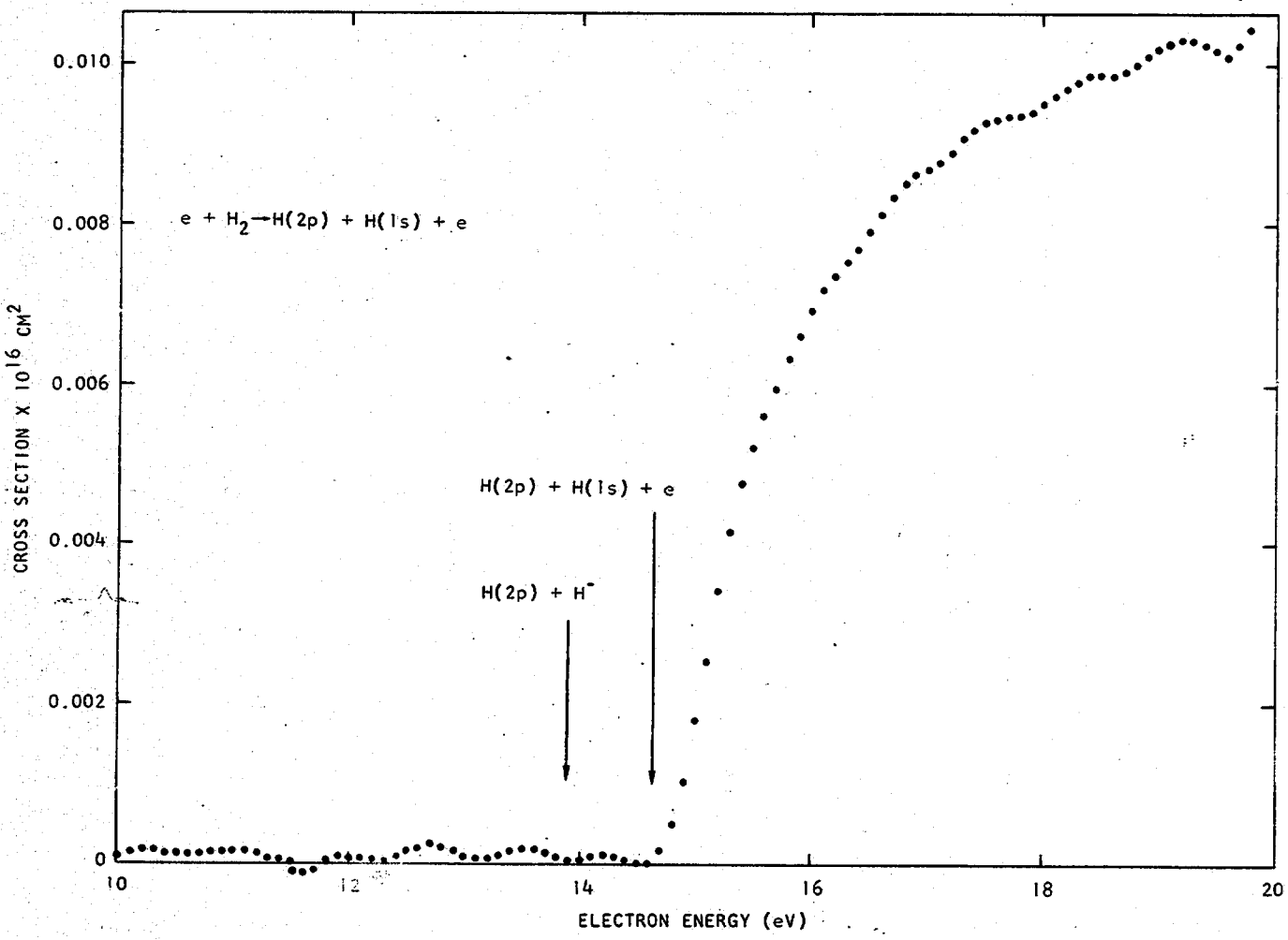



**Fig. 10.** The excitation curve for dissociative excitation resulting from the removal of the molecular contribution below 14 eV. This curve is generated by subtracting ~5% of the helium signal from the $O_2$ curve

## 7. DISSOCIATIVE EXCITATION OF MOLECULAR HYDROGEN

From the discussion in Section 6, it is clear that the originally reported value for the dissociative excitation of the 2p state of atomic hydrogen from $H_2$ was in error due to a large contribution of molecular radiation coming from the interaction region. As can be seen in Fig. 11, the cross section for $H_2$ is nearly 20% lower than the original measurements of Fite and Brackmann.[1] It is also clear from Fig. 11 that the dissociative excitation of $D_2$ has a cross section that is only 90% of that of $H_2$. This isotope effect is in keeping with the predictions of Platzman,[11] who pointed out that there are a number of molecular states that lie above the first ionization potential. In general, there are two major deexcitation paths available for such excited states, autoionization and predissociation. The first of these processes is nearly mass independent; the time for it therefore should almost be independent of isotope substitution. The time required for dissociation depends on the velocity with which the particles separate and therefore is strongly mass dependent. A similar isotope effect has recently been reported by Burrows and Dunn[12] and by Vroom and deHeer.[13] Shown also in Fig. 11 is the maximum of the Balmer-alpha excitation curve of Burrows and Dunn. The shape of the curve is very similar to our $H_2$ curve.

In our preliminary data, the break in the total excitation curve in the case of $H_2$ is at a higher potential than in the case of $D_2$. It is clear from the figure that in the case of $D_2$ the channel that includes excitation plus proton formation does not play a major role, whereas in the case of $H_2$ the onsets of both the formation of two excited states and the formation of the (2p) atom plus a proton are below the major structure that appears in our curve. No doubt this is associated with the isotope effect, details of which are not yet completely understood.

In Fig. 12 we show the excitation curve near threshold. The data shown are only relative. This curve is one from which the energy distribution of our beam has been largely removed. Three sets of data are overlapped. The structure that appears at the end of the first also appears in the beginning of the second; similarly, the structure that appears at the end of the second appears in the beginning of the third. The onset is in the vicinity of 14.7 eV. There follows a rather straight portion of the curve with very little structure. Then, in the vicinity of 15.8 eV the onset of nearly 12 small ripples, which are fairly evenly spaced, is seen. The spacing between the

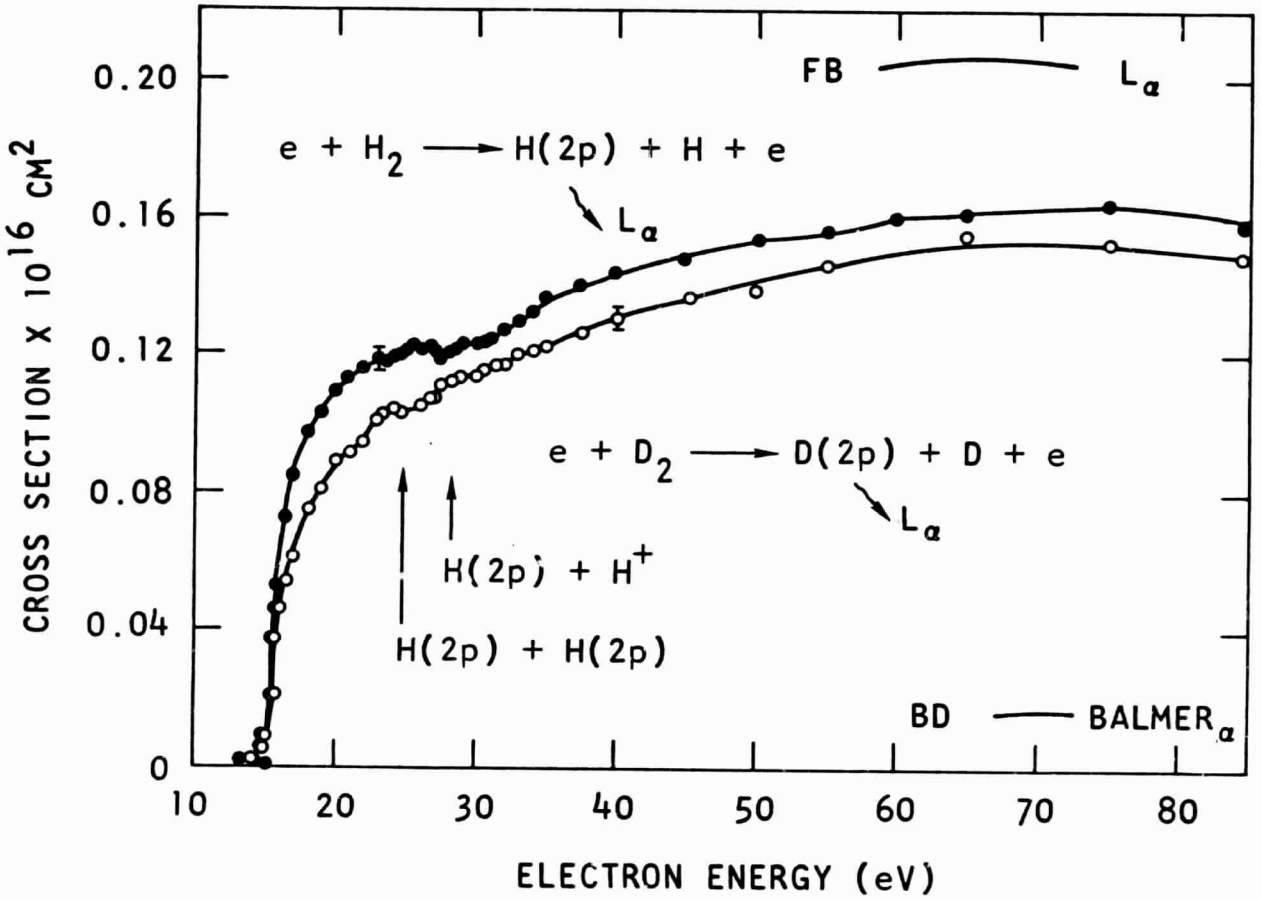



Fig. 11. A comparison of the dissociative excitation results for $H_2$ and $D_2$. Also shown are a segment from the earlier Lyman-alpha excitation measurements of Fite and Brackmann (FB) and a segment of the Balmer-alpha excitation curve of Burrows and Dunn (BD)

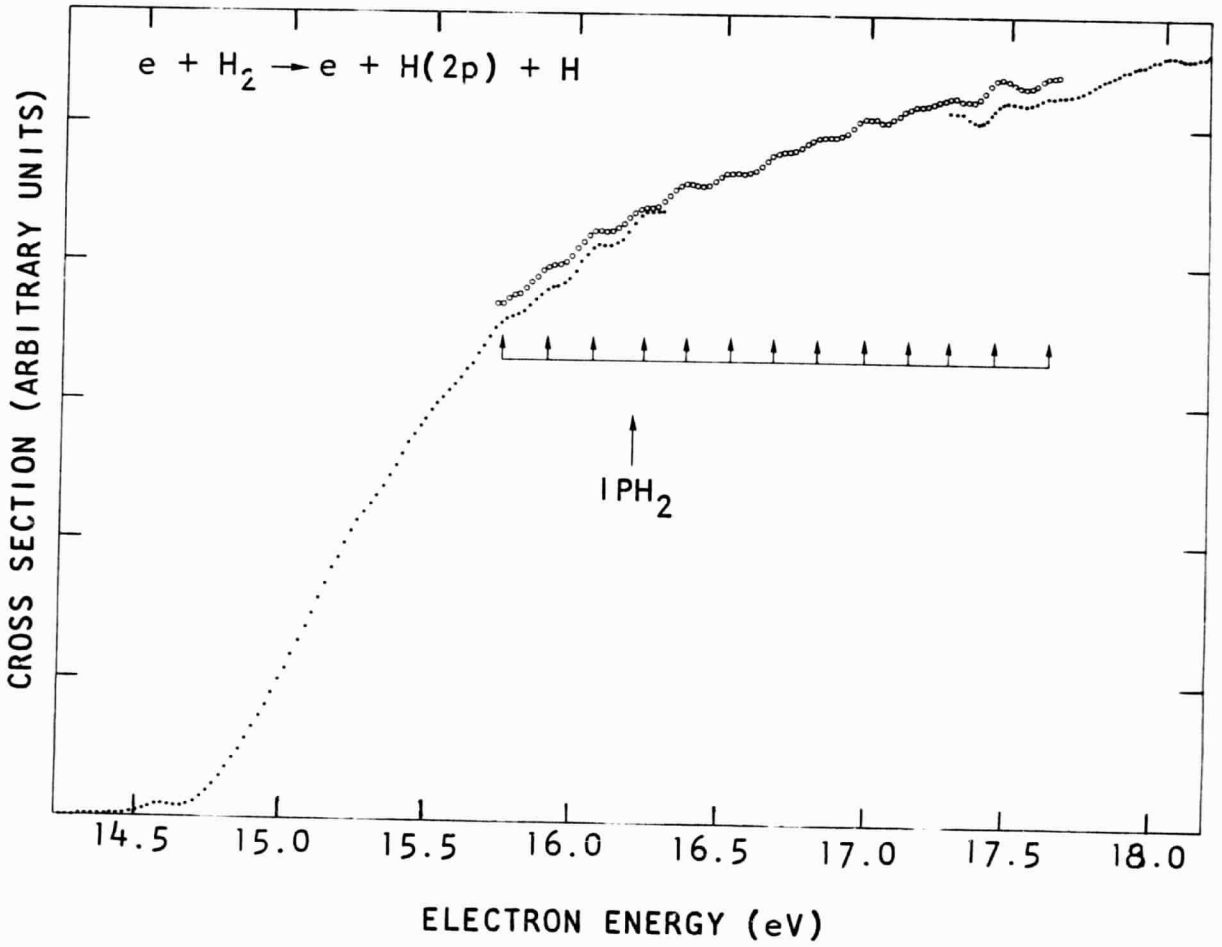



Fig. 12 A segment of the dissociative excitation curve near threshold, from which much of the 0.07-eV electron energy distribution is analytically removed from the curve

ripples is in the vicinity of 0.14 to 18 eV. This series of ripples shows a change above the ionization potential, 15.43 eV. In fact, the continuous ripple form goes on until nearly 17.8 eV, the dissociation limit of $H_2^+$. Above this the nature of the structure changes, and the orderliness seems to disappear. The larger ripples which are apparent in Fig. 10 then seem to dominate. The cause of this structure is not completely understood. It is possible, although not likely, that it is due to the structure in the molecular radiation in the background of our signal, which has not been completely removed. If, however, this structure is related to the dissociative excitation of $H_2$ into the 2p channel, then one is prompted to suggest either that it results from a temporary formation of an $H_2^-$ compound state, which decays into several modes, one the dissociative channel and the other the excitation of molecular levels, or that it reflects competition between predissociation and autoionization, i.e.,

$$e + H_2 \rightarrow H_2^* + e ,$$

followed by

$$H_2^* \rightarrow H(2p) + H(1s)$$

competing with

$$\rightarrow H_2^* + e .$$

## 8. THE THEORETICAL COMPLEMENT

During this contract period, Professor J. C. Y. Chen, University of California, San Diego (UCSD), has participated in our study of electron hydrogen collisions. His activities at Gulf General Atomic and at the University have covered the following subjects:

1. The application of Faddeev's equation to a number of atomic problems
   a. (e-H) elastic scattering resonances
   b. (e-H) excitation threshold
   c. ($e^+$-H) elastic scattering and positronium formation
2. Close-coupling calculations (or the (e-H) system in momentum space)
3. Electron resonance scattering from molecules

Work is also under way at UCSD on a new variational calculation for (e-H) scattering and on the field detachment of $H^-$.

Included in Appendix II is an article that resulted from these studies. In it, Ball, Chen, and Wong have investigated various solutions of the Faddeev equation for Coulomb potentials, and a practical method for solving the Faddeev equations below the three-particle breakup threshold is developed. The method is then applied to the (e, H) system in which the $H^-$ bound state and the lowest members of the compound states in both the singlet and triplet series are calculated. The calculated position of the lowest $^1S$ resonance is in excellent agreement with the experiment, while the width of the lowest $^1S$ resonance is slightly less than that found experimentally.

Also during this contract year, with the support of NASA and Gulf General Atomic, a series of colloquia on atomic and molecular processes (CAMP) has been conducted. Many of the colloquia were given by people who are actively participating in electron proton and positron hydrogen atom scattering studies. A list of colloquia speakers and their topics is given in Section 10.

This spring a two-day "working session" on electron hydrogen atom collisions was held in La Jolla. The primary purpose of this session was to consider the programs presently under way and to determine what information could best be obtained from experiment to direct further theoretical studies. The program for this successful working session is also listed in Section 10.

# 9. DATA PROCESSING FOR ELECTRON-ATOM ELASTIC AND INELASTIC EXPERIMENTS AND A PROGRAM LISTING

The output data from the experimental devices are on punched paper tape. In order to process these data using the 1108 FORTRAN IV programs, the data first must be converted to punched cards or magnetic tape. Because of the ease in handling, storing, etc., the latter was chosen. To aid in understanding the descriptions and the instructions for the use of the various programs involved, a brief listing of terms and definitions is presented below.

## 9.1. TERMINOLOGY

### Paper Tape

Data word: a fixed number of digits plus separator character

Data block: a block consisting of four data words--channel chamber, signal + noise, noise, and current, respectively

Data section: a section of paper tape that contains a finite number of data blocks

Leader: a section of paper tape that is comprised of feed characters

Illegal character: any punch or combination of punches that does not represents digits 0 through 9, a separator, or a feed character

### Magnetic Tape

FD (Field Data Code): 2 octal digit code representation for character and digit

Floating point: the form in which a number containing an implied decimal must be before computation in FORTRAN IV can take place with meaningful results

Image tape: magnetic tape on which the image of a paper tape is written, except illegal characters, which are represented as slashes (/) (FD format)

Library tape: magnetic tape in which many data sections are stored for later retrieval

Scratch tape: tape used for one computer run only; its contents are not saved

Backup tape: a copy of any magnetic tape, used for protection purposes

## 9.2. PAPER TAPE FORMAT

The paper tape must contain a minimum of five feet of leader before the first data section. The leader must be marked "START" in large letters. Each data section must be separated by a minimum of 18 inches of feed characters. Five feet of leader must follow the last data section.

## 9.3. DESCRIPTION AND INSTRUCTIONS

This section contains a description of the function of each of the following programs used in conjunction with the electron scattering experiments, along with a detailed set of directions for use and a listing of the complete program for each.

| Program Name | Program Function |
|---|---|
| 1. READPT | Used with the 1004 paper tape reader to read the paper tape and write the information on a magnetic tape. A slash (/) is written on the magnetic tape for any illegal character in the paper tape. |
| 2. TEDIT | Reads the magnetic tape as written by READPT, converts data from FD to floating point format, and stacks information on a library data tape. Output consists of printed tape and printer plots. Eliminates any illegal characters (slashes) by linear interpolation or direct substitution. |
| 3. TREAD | Reads the data library tape written by TEDIT and lists all runs on this tape. |
| 4. ABEAM4 | Reads the data library tape written by TEDIT and provides various calculations and printer plots as requested by user. |
| 5. COPY | Reads the data library tape and copies the information onto backup tape. |

6. UPDATE — Allows the user to make certain changes to the data on the library tape. A new library tape is written and the original library tape remains unchanged.

7. LEØF — Reads the data library tape, lists all experiments by number, and writes end of file on the tape. (It was designed to place an end of file on the library tape when it was omitted by TEDIT through oversight on the part of user or through a fault of the computer during a TEDIT run.)

8. SMØØTH — Fourier-smooths data, unfolds a given Gaussian electron energy distribution from the data, and gives the results in tabular form. At present only the derivatives of the data are given. The program is prepared to accept card input. The deck of cards needed is generated as one of the options in ABEAM4.

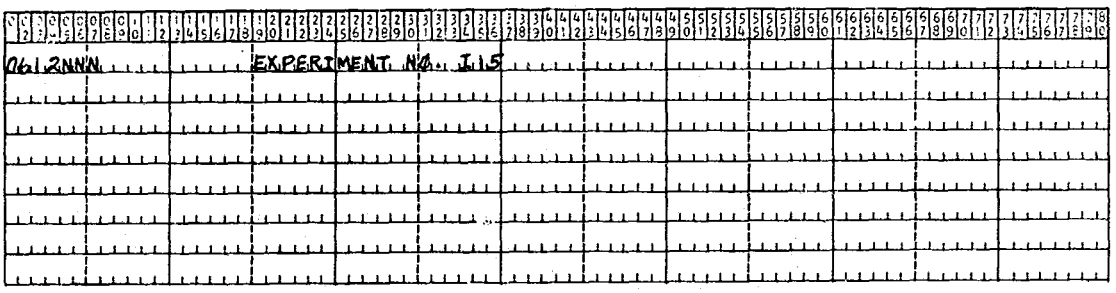
9. SIMCUR — Folds into any given function a Gaussian distribution of specified full width at half maximum. The results are generated in both tabular and graphic form.

10. SIMTAB — Folds into any function in tabular form a Gaussian distribution of specified full width at half maximum. A ninth-order polynomial interpolation scheme is included in this program. The results are given in both tabular and graphic form.

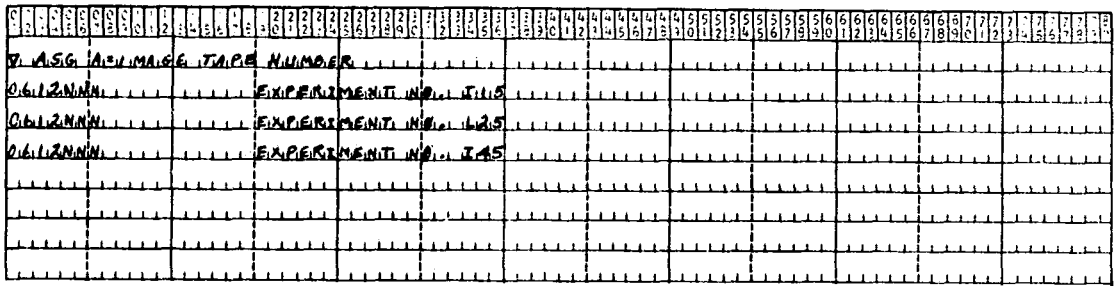
STEP 1: READPT

The information contained on the paper tape is transferred to a magnetic tape by the READPT program. The READPT program is an integral part of the 1108 system; therefore, no program deck is required by the user.

The paper tape must be in the format described in Section 9.2. A data card must be punched for each data section on the paper tape to be read by READPT. The format of the data card is as follows:



The information in columns 1 through 7 is mandatory. The information starting in column 19 for identification of each data section is arbitrary. Below is an example READPT input deck for a paper tape containing three data sections.




The printed output from READPT consists of three data blocks per line. Slashes are substituted for any illegal characters in the paper tape.

Prior to the start of step 2, the TEDIT program, the output listing from READPT is examined for errors. A data section is made up of one or more cycles. The channel numbers normally run sequentially, starting at 00000, to a maximum of 00099 for each cycle. In order for TEDIT to recognize the start of a new cycle it is mandatory that each starting channel number be all zeros (00000) and contain no slashes. TEDIT will correct all other channel numbers that contain slashes.

On the output listing from READPT, columns 1, 5, and 9 are the channel numbers. If errors in the paper tape have caused the channel numbers to shift from these columns, the paper tape must be corrected and step 1 repeated until all errors of this type have been eliminated.

The computer program is not included in this report since it is a standard library program held at the computer center.

STEP 2: TEDIT

TEDIT reads a data card, then reads a data section from the magnetic tape written by READPT. It converts the tape data from FD to floating point and a fixed point (integer) and writes the information on the library tape (to be used by ABEAM4 program). The printed output from TEDIT contains the following:

1. A listing of each data section by cycle
2. A printer plot of (signal + noise) - (noise) = signal
3. A printer plot of current by cycle
4. After processing each data section, a listing of $\Sigma^*$ signal, $\Sigma$(signal + noise), $\Sigma$ noise, $\Sigma$(signal/current), $\Sigma$((signal + noise)/current), $\Sigma$(noise/current) is given. Also, a printer plot of $\Sigma$ signal and $\Sigma$(signal/current) is given.

When a blank data card is encountered, an end of file is written on the library tape and processing is completed.

The data card for each data section must be in the following format:

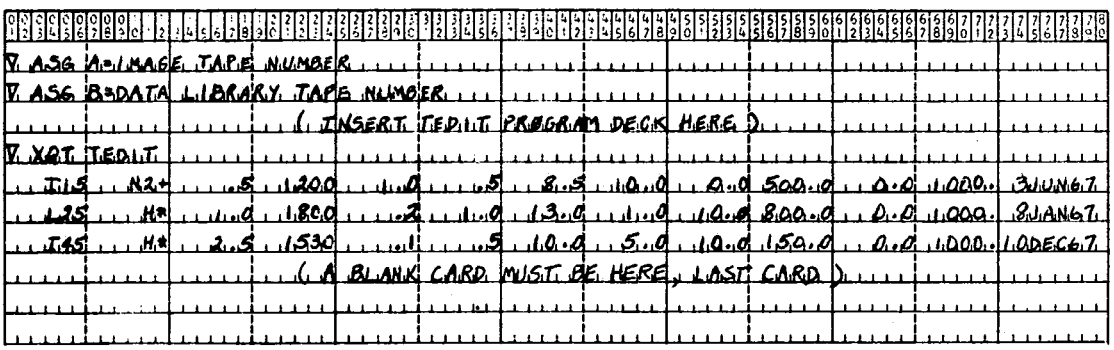
| Column | Name of Variables | FORTRAN Format |
|---|---|---|
| 1-6 | Experiment number | A6 |
| 7-12 | Gas type | A6 |
| 13-18 | Current variance | F6.0 |
| 19-24 | Time of starting experiment | A6 |
| 25-30 | Resolution | F6.0 |
| 31-36 | Voltage interval | F6.0 |
| 37-42 | Initial voltage | F6.0 |
| 43-48 | Time interval (sec) | F6.0 |
| 49-54 | Approximate minimum signal | F6.0 |
| 55-60 | Approximate maximum signal | F6.0 |
| 61-66 | Approximate minimum current | F6.0 |
| 67-72 | Approximate maximum current | F6.0 |

*$\Sigma$ is defined as the summing of each respective channel number over all cycles.

| | | |
|---|---|---|
| 73-79 | Date of experiment | A6, A1 |
| 80 | When a new library tape is to be created, a one (1) must be punched in column 80 of the first data card only. Otherwise, this column is left blank. | I1 |

Data cards must be in the same sequence as the experiments (data sections) on the paper tape. The information from the data cards is also written on the library tape (except column 80).

Below is an example deck setup consisting of three experiments. The last card must be a blank card.




On the 1108 run request form, check "Do Not Rerun This Job." The number of experiments that may be stacked on the data library tape depends on tape size; the maximum number is 200.

A program listing follows.

```
@ FOR TEDIT,TEDIT
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4614B
THIS COMPILATION WAS DONE ON 02 MAY 68 AT 10:19:07

   MAIN PROGRAM          ENTRY POINT 000000

 1.    C.. THE PURPOSE OF THIS ROUTINE IS TO READ A MAG. TAPE CONTAINING THE
 2.    C   IMAGE OF ONE OR MORE PAPER TAPES. EDIT THIS TAPE AND WRITE THE INFO.
 3.    C   ON A LIBRARY DATA TAPE.
 4.    C
 5.          DIMENSION CHAN(100), SPLUSN(100), NOISE(100), CURR(100), SIG(100),
 6.         1   X(102), Y(102)
 7.          REAL NOISE
 8.          INTEGER CHAN
 9.          DIMENSION ERR1(100), ERR2(100), ERR3(100), ERR4(100), BUFF(90),
10.         1 WORD(72), ERROR(12), DATE(2)
11.          DIMENSION SUM1(100), SUM2(100), SUM3(100), SUM4(100), SUM5(100),
12.         1          SUM6(100)
13.          PARAMETER PTAPE = 9, LTAPE = 10
14.          INTEGER BUFF, BLANK, SLASH, FIVE, ASTER, ERROR, ERR1, ERR2, ERR3,
15.         1   ERR4, TEE
16.          COMMON BUFF
17.          DATA BLANK/6H     /, SLASH/6H/     /, FIVE/6H5     /, ASTER/6H *
18.         1   /, MINUS/6H-     /, TEE/6HT     /
19.          REWIND PTAPE
20.          REWIND LTAPE
21.          IBEGIN = 0
22.    C..   READ MAIN DATA CARD, ONE PER EACH PAPER TAPE IMAGE ON MAG. TAPE (PTAPE).
23.       10 READ(5,11) NUM, ITYPE, VAR, TIME, RES, DVOLT, VOLTST, TINT, SIGMIN
```

```
      1 , SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2), ITIME
   11 FORMAT( 2A6, F6.0, A6, 8F6.0, A6, A1, I1 )
C.. HAS THE LAST PAPER TAPE IMAGE BEEN PROCESSED?
      IF(NUM.NE.BLANK) GO TO 14
   12 CALL REWI(LTAPE)
      CALL REWI (PTAPE)
      STOP
C.. INITIALIZE CYCLE COUNTER TO ZERO, SET LAST CYCLE FLAG TO ZERO.
   14 KOUNT = 0
      DO 15 I=1,100
      SUM1(I) = 0.0
      SUM2(I) = 0.0
      SUM3(I) = 0.0
      SUM4(I) = 0.0
      SUM5(I) = 0.0
   15 SUM6(I) = 0.0
C.. SET INDEX COUNTER FOR CHAN, SPLUSN, NOISE AND CURR ARRAYS TO ZERO.
      L = 0
      WRITE(6,17) NUM, ITYPE, VAR, TIME, RES
   17 FORMAT( 1H1, 9X 10HRUN NUMBER, 1X, A6, // 10X 3HGAS 1X A6,// 10X
     1 10HVARIANCE %, 1X F6.2, // 10X 4HTIME, 1X A6, // 10X 4HRES. 1X
     2 F6.2 / )
      WRITE(6,18) DVOLT, VOLTST, TINT, SIGMIN, SIGMAX, CURMIN, CURMAX
   18 FORMAT( 10X 17HVOLTAGE INCREMENT 1X F6.2, // 10X 17HSTARTING VOLTA
     1GE  1X F6.2, // 10X 14HTIME INTERVAL , F6.2, // 10X 12HMIN. SIGNAL
     2  F10.2, // 10X 12HMAX. SIGNAL ,F10.2, // 10X 13HMIN. CURRENT ,
     3 F10.2, // 10X 13HMAX. CURRENT , F10.2, / )
```

```
      WRITE(6,19) DATE(1), DATE(2)
   19 FORMAT( 10X, 4HDATE, 1X 2A6, / )
   30 WRITE(6,31)
   31 FORMAT( 1H1 )
C.. INCREMENT CYCLE COUNTER BY ONE.
      KOUNT = KOUNT + 1
C.. READ ONE RECORD FROM PTAPE.
   40 READ(PTAPE,41) (BUFF(I), I=1,90)
   41 FORMAT( 90A1 )
C.. TRANSLATE RECORD..
      CALL GINPUT ( WORD, N )
      DO 45 I=1,12
   45 ERROR(I) = BLANK
C.. IF THERE WERE ILLEGAL CHARACTERS IN THE RECORD GO TO 50.
      IF(N.EQ.72) GO TO 50
C.. WAS THIS RECORD AN END FILE, ALL BLANKS.
      IF(N.NE.0)  GO TO 80
      ISWTCH = 1
      GO TO 140
C..   BEGIN TESTING THE LEGALITY OF EACH CHARACTER.
   50 DO 70 I=1,72
      IF(MOD(I,6).EQ.0) GO TO 60
      IF(BUFF(I).NE.SLASH.AND.BUFF(I).NE.TEE) GO TO 70
      BUFF(I) = FIVE
      K = I/6 + 1
C.. FLAG K WORD IN RECORD TO BE IN ERROR.
      ERROR(K) = ASTER
```

```
      GO TO 70
   60 IF(BUFF(I).EQ.BLANK) GO TO 70
      BUFF(I) = BLANK
   70 CONTINUE
C.. RETRANSLATE RECORD, RECORD NOW CONTAINS DIGITS AND BLANKS ONLY, NO SLASHES.
      CALL GINPUT ( WORD, N )
C.. SEE IF A NEW CYCLE IS STARTING WITHIN LAST TRANSLATED RECORD, WORD(1),
C   WORD(5) OR WORD(9) WILL EQUAL ZERO.
   80 IF(L.EQ.0.AND.KOUNT.EQ.1) GO TO 100
      IF(N.GT.4) GO TO 82
      N = 4
      GO TO 85
   82 IF(N.GT.8) GO TO 84
      N = 8
      GO TO 85
   84 N = 12
   85 DO 90 K=4,N,4
      J = K-3
      IF(WORD(J)) 90, 120, 90
   90 CONTINUE
C.. NO NEW CYCLE PLACE ALL WORDS INTO PROPER ARRAYS.
      JSAVE=0
  100 DO 110 J =1,N,4
      L = L + 1
C.. TEST FOR EXCEEDING RESERVED STORAGE.
      IF(L.GT.100) GO TO 300
      CHAN(L) = WORD(J) + .5
```

```
105.          SPLUSN(L) = WORD(J+1)
106.          NOISE(L)  = WORD(J+2)
107.          CURR(L)   = WORD(J+3)
108.          ERR1(L)   = ERROR(J)
109.          ERR2(L)   = ERROR(J+1)
110.          ERR3(L)   = ERROR(J+2)
111.      110 ERR4(L)   = ERROR(J+3)
112.          GO TO 40
113.    C.. A NEW CYCLE STARTS WITHIN LAST RECORD.
114.      120 ISWTCH = 0
115.          JSAVE = J
116.          IF(JSAVE.EQ.1) GO TO 140
117.          K = JSAVE - 4
118.          DO 130 J=1,K,4
119.          L = L + 1
120.    C.. TEST FOR EXCEEDING RESERVED STORAGE.
121.          IF(L.GT.100) GO TO 300
122.          CHAN(L) = WORD(J) + .5
123.          SPLUSN(L) = WORD(J+1)
124.          NOISE(L)  = WORD(J+2)
125.          CURR(L)   = WORD(J+3)
126.          ERR1(L)   = ERROR(J)
127.          ERR2(L)   = ERROR(J+1)
128.          ERR3(L) = ERROR(J+2)
129.      130 ERR4(L) = ERROR(J+3)
130.    C.. TEST EACH ERROR FLAG, IF CHAN(I) IS IN ERROR SUBSTITUTE I-1.
131.    C                         IF SPLUSN(I), NOISE(I) OR CURR(I) IS IN ERROR
```

```
C                          INTERPOLATE FOR ITS VALUE.
  140 DO 180 I=1,L
      IF(ERR1(I).NE.BLANK) CHAN(I) = I-1
      IF(I.NE.1) GO TO 150
      I1 = 2
      I2 = 3
      GO TO 170
  150 IF(I.NE.L) GO TO 160
      I1 = L-2
      I2 = L-1
      GO TO 170
  160 I1 = I-1
      I2 = I+1
  170 IF(ERR2(I).EQ.BLANK) GO TO 172
      SPLUSN(I) = (SPLUSN(I2)-SPLUSN(I1))*FLOAT(I-I2)/FLOAT(I2-I1) +
     1  SPLUSN(I2)
  172 IF(ERR3(I).EQ.BLANK) GO TO 174
      NOISE(I) = (NOISE(I2)-NOISE(I1))*FLOAT(I-I2)/FLOAT(I2-I1) +
     1  NOISE(I2)
  174 IF(ERR4(I).EQ.BLANK) GO TO 180
      CURR(I) = (CURR(I2)-CURR(I1))*FLOAT(I-I2)/FLOAT(I2-I1) + CURR(I2)
  180 CONTINUE
C     UPDATE LTAPE WITH THIS CYCLE DATA.
      IF(IBEGIN.NE.0) GO TO 182
      IBEGIN = 1
      IF(ITIME.EQ.1) GO TO 184
      CALL NTRAN(LTAPE, 8, 1, 8, -1)
```

```
      BACKSPACE LTAPE
      GO TO 183
  182 CALL NTRAN(LTAPE, 8, -1)
      BACKSPACE LTAPE
      IF(KOUNT.GT.1) GO TO 185
  183 LAST = 1
      WRITE(LTAPE) LAST
  184 WRITE(LTAPE) NUM, ITYPE, VAR, TIME, RES, DVOLT, VOLTST, TINT,
     *  SIGMIN, SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
      GO TO 186
  185 LAST = 0
      WRITE(LTAPE) LAST
  186 WRITE(LTAPE) KOUNT, L
      WRITE(LTAPE) (CHAN(I), SPLUSN(I), NOISE(I), CURR(I), I=1,L)
      LAST = 2
      WRITE(LTAPE) LAST
      END FILE LTAPE
C     CALCULATE SIGNAL VALUE FOR PLOTTING.
      X(1) = VOLTST
      X(L+2) = VOLTST + FLOAT(L-1)*DVOLT
      Y(1)   = SIGMIN
      Y(L+2) = SIGMAX
      DO 190 I=1,L
      X(I+1) = VOLTST + FLOAT(I-1)*DVOLT
      SIG(I) = SPLUSN(I) - NOISE(I)
      SUM1(I) = SUM1(I) + SIG(I)
      SUM2(I) = SUM2(I) + SPLUSN(I)
```

```
      SUM3(I) = SUM3(I) + NOISE(I)
      SUM4(I) = SUM4(I) + SIG(I)/CURR(I)
      SUM5(I) = SUM5(I) + SPLUSN(I)/CURR(I)
      SUM6(I) = SUM6(I) + NOISE(I)/CURR(I)
  190 Y(I+1) = SIG(I)
  200 WRITE(6,201) NUM, KOUNT
  201 FORMAT( 30X, 14HPLOT OF SIGNAL  5X 4HRUN  A6, 5X 5HCYCLE, I3 )
C.. PLOT VALUES OF SIGNAL.
      CALL PLOT( X, Y, L+2, 102, 46, 6 )
C.. PLOT VALUES OF CURRENT.
      WRITE(6,31)
      WRITE(6,202) NUM, KOUNT
  202 FORMAT( 30X, 15HPLOT OF CURRENT 5X 4HRUN  A6, 5X 5HCYCLE, I3 )
      Y(1)   = CURMIN
      Y(L+2) = CURMAX
      DO 203 I=1,L
  203 Y(I+1) = CURR(I)
      CALL PLOT( X, Y, L+2, 102, 46, 6 )
C.. LIST ALL DATA FOR THIS CYCLE.
      WRITE(6,31)
      WRITE(6,204) NUM, KOUNT
  204 FORMAT( 22X, 4HRUN  A6, 5X 5HCYCLE, I3, //   ,6X 5HCHAN, 5X 3HS+N,
     1  9X 1HN, 10X, 1HI, 10X, 1HS /)
      WRITE(6,206) (ERR1(I), CHAN(I), ERR2(I), SPLUSN(I), ERR3(I),
     1  NOISE(I), ERR4(I), CURR(I), SIG(I),  I=1,L )
  206 FORMAT( 14X, A2, I3, 2X, A2, F7.0, 2X, A2, F7.0, 2X, A2, F7.0,
     1  4X, F10.3 )
```

```
      WRITE(6,208)
  208 FORMAT( 6X, 66H* INDICATES THE VALUE TO THE RIGHT CONTAINED AN ILL
     1EGAL CHARACTER. / 8X 36HTHE NEW VALUE HAS BEEN INTERPOLATED.  )
C.. TEST FOR END OF PAPER TAPE IMAGE.
      IF(ISWTCH.NE.0) GO TO 240
C.. PREPARE FOR A NEW CYCLE ON PRESENT PAPER TAPE IMAGE.
C.. RESET INDEX COUNTER FOR CHAN, SPLUSN, NOISE AND CURR ARRAYS TO ZERO.
      L = 0
      IF(JSAVE.EQ.0) GO TO 30
      DO 210 I=JSAVE,N,4
      L = L + 1
C.. TEST FOR EXCEEDING RESERVED STORAGE.
      IF(L.GT.100) GO TO 300
      CHAN(L) = WORD(I) + .5
      SPLUSN(L) = WORD(I+1)
      NOISE(L)  = WORD(I+2)
      CURR(L)   = WORD(I+3)
      ERR1(L) =  ERROR(I)
      ERR2(L) =  ERROR(I+1)
      ERR3(L) =  ERROR(I+2)
  210 ERR4(L) =  ERROR(I+3)
      GO TO 30
C.. END OF THIS PAPER TAPE IMAGE.
C..   PLOT VALUES FOR SUMMATION OF SIGNAL VS. VOLTS.
  240 WRITE(6,31)
  260 WRITE(6,261) NUM
  261 FORMAT( 30X 27HPLOT OF SUMMATION OF SIGNAL 5X 3HRUN A6 )
```

```
      CALL PLOT ( X, SUM1, L, 100, 46, 6 )
      WRITE(6,31)
C,,   PLOT VALUES FOR SUMMATION OF SIGNAL/CURRENT VS. VOLTS.
      WRITE(6,291) NUM
  291 FORMAT( 30X 35HPLOT OF SUMMATION OF SIGNAL/CURRENT  5X 3HRUN A6 )
      CALL PLOT ( X, SUM4, L, 100, 46, 6 )
      WRITE(6,31)
      WRITE(6,292) NUM
  292 FORMAT( 50X 3HRUN A6, 5X 23HSUMMATION OF ALL CYCLES // 5X 5HCHAN.
     1  10X 5HVOLTS 12X 1HS 13X 3HS+N 13X 1HN 13X 3HS/I 9X 7H(S+N)/I
     2  11X 3HN/I  / )
      WRITE(6,293) (CHAN(I), X(I+1), SUM1(I), SUM2(I), SUM3(I), SUM4(I),
     1              SUM5(I), SUM6(I), I=1,L )
  293 FORMAT( I8, 4X, 1P7E15.4  )
      GO TO 10
  300 WRITE(6,301) NUM, KOUNT
  301 FORMAT( 1H1, 14H **ERROR** RUN, A6, 3X, 5HCYCLE, I6, 33H CONTAINS
     1MORE THAN 100 CHANNELS. / 27H REMAINDER OF DATA IGNORED. )
      GO TO 12
      END
END OF LISTING.    0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR GINPUT,GINPUT
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 02 MAY 68 AT 10:19:11

    SUBROUTINE GINPUT    ENTRY POINT 000314
 1.         SUBROUTINE GINPUT ( WORD, N )
 2.    C.. THIS ROUTINE IS A MODIFIED VERSION OF GINPUT.
 3.    C.. THE FOLLOWING MODIFICATIONS WERE MADE,
 4.    C   1) COL IS NOW IN COMMON.
 5.    C   2) STATEMENTS 5 AND 6 ARE NOW COMMENTS.
 6.    C.. THE PURPOSE OF THIS ROUTINE IS TO READ 72 COLUMNS OF FREE FORMATED
 7.    C   INFORMATION ON A CARD,  DATA MUST BE SEPERATED BY A BLANK OR COMMA.
 8.    C.. WORD IS THE ARRAY IN WHICH THIS ROUTINE STORES THE CARD INFORMATION.
 9.    C   IT MUST BE DIMENSION 72 IN THE MAIN PROGRAM FOR ALPHA-NUMERIC INFO.
10.    C   TITLE CARDS ARE THEN WRITTEN USING 72A1 FORMAT.
11.    C.. N WILL INDICATE THE FOLLOWING TO THE MAIN PROGRAM...
12.    C       1) N = 72 , CARD WAS ALPHA-NUMERIC.
13.    C       2) N =-72 , CARD WAS ALL BLANK EXCEPT FOR AN EQUAL SIGN.
14.    C       3) 0<N<72 , CARD CONTAINED N FLOATING POINT VALUES, THE FIRST IS
15.    C                   STORED IN WORD(1), SECOND ONE IN WORD(2), ETC.
16.    C       4) -72<N<0, SAME AS 3) EXCEPT AN EQUAL SIGN WAS FOUND AT LEAST
17.    C                   ONE SPACE BEYOUND THE LAST FLOATING POINT NUMBER.
18.    C       5) N = 0    ALL BLANK CARD.
19.    C.. IF A CHARACTER OTHER THAN A PLUS OR MINUS SIGN, COMMA, BLANK, DIGIT,
20.    C   DECIMAL POINT OR EQUAL SIGN IS DETECTED ON A CARD THEN THE CARD IS
21.    C   INTERPRETED AS ALPHA-NUMERIC IMEDIATELY.
22.    C.. THE PURPOSE OF THE EQUAL SIGN IS TO SERVE AS A FLAG FOR WHATEVER THE
```

```
C   USER WISHES.
C.. THE FORTRAN E FORMAT IS NOT ALLOWED. THE LARGEST ALLOWABLE NUMBER IS
C   9999999999. OR 9X10**9.
      INTEGER COL, TESTWD
      DIMENSION WORD(72), TESTWD(16), COL(72), FWORD(72)
      COMMON COL
      EQUIVALENCE ( FWORD, COL )
      DATA (TESTWD(I),I=1,16)/1H0, 1H1, 1H2, 1H3, 1H4, 1H5, 1H6, 1H7,
     1 1H8, 1H9, 1H , 1H+, 1H., 1H=, 1H-, 1H* /
C   5 READ 6, ( COL(I), I=1,72 )
C   6 FORMAT( 72A1 )
      K = 0
      N = 0
      SUM = 0.0
      DEC = 0.0
      IGO = 1
    8 SIGN = 1.0
C.. FIND FIRST NON-BLANK CHARACTER.
      DO 7 I=1,72
      IF(COL(I).NE.TESTWD(11)) GO TO 11
    7 CONTINUE
      N = 0
      GO TO 16
C.. BEGIN TESTING AT START OF NEW WORD.
   10 IF(COL(I).EQ.TESTWD(11)) GO TO 20                    BLANK
   11 IF(COL(I).EQ.TESTWD(15)) GO TO 30                    MINUS
```

```
      IF(COL(I).EQ.TESTWD(16)) GO TO 40                    PLUS
      IF(COL(I).EQ.TESTWD(13)) GO TO 50                    DECIMAL
      DO 12 J=1,10
      IF(COL(I).EQ.TESTWD(J) ) GO TO 60                    0 THRU 9
   12 CONTINUE
      IF(COL(I).EQ.TESTWD(12)) GO TO 70                    COMMA
   15 IF(COL(I).EQ.TESTWD(14)) GO TO 80                    EQUAL
C.. CHARACTER WAS ALPHA-NUMBERIC.
      N = 72
   16 DO 17 I=1,72
   17 WORD(I) = FWORD(I)
   18 RETURN
   20 GO TO(22, 18),IGO
   22 I = I + 1
      IF(I-72) 10, 10, 18
C
   30 SIGN = -1.0
C.. CHARACTER WAS A MINUS SIGN.
      GO TO 22
C
   40 SIGN = +1.0
C.. CHARACTER WAS A PLUS SIGN.
      GO TO 22
C
   50 K = -1
C.. CHARACTER WAS A DECIMAL POINT.
```

```
      KSAVE = 0
C.. INDICATE DECIMAL WAS FOUND.
      DEC = 1.0
      GO TO 100
C
   60 K = 10
C.. CHARACTER WAS A DIGIT.
C   ASSUME WORD HAS 10 SIGNIFICANT DIGITS TO THE LEFT OF THE DECIMAL.
      GO TO 120
C
C.. CHARACTER WAS A COMMA PRECEDED BY BLANKS OR ANOTHER COMMA.
   70 N = N + 1
      WORD(N) = 0.0
      I = I + 1
      GO TO 10
C
C.. CHARACTER WAS AN EQUAL SIGN.
   80 IF(N) 84, 82, 84
   82 N = -72
      RETURN
   84 N = -N
      RETURN
C
  100 I = I + 1
C
      IF(I-72) 110, 110, 105
```

```
C.. INDICATE ENTIRE RECORD HAS BEEN TRANSLATED.
  105 IGO =2
      GO TO 135
  110 DO 112 J=1,10
      IF(COL(I).EQ.TESTWD(J) ) GO TO 120                    0 THRU 9
  112 CONTINUE
      IF(COL(I).EQ.TESTWD(13)) GO TO 130                    DECIMAL
      IF(COL(I).EQ.TESTWD(12)) GO TO 135                    COMMA
      IF(COL(I).EQ.TESTWD(11)) GO TO 135                    BLANK
      GO TO 10
C
C.. BUILD UP WORD BY ADDING ON DIGIT JUST FOUND.
  120 SUM = SUM + FLOAT(J-1)*10.0**K
      K = K - 1
      GO TO 100
C
C.. SAVE POSITION WHERE DECIMAL WAS FOUND.
  130 KSAVE = K + 1
C.. INDICATE THAT DECIMAL WAS FOUND.
      DEC = 1.0
      GO TO 100
C
C.. ALTER CHARACTERISTIC OF FLOATING POINT WORD FOR DECIMAL POINT.
C.. SEE IF A DECIMAL POINT WAS FOUND.
  135 IF(DEC) 140, 138, 140
  138 KSAVE = K + 1
```

```
C.. UPDATE WORD COUNTER.
  140 N = N + 1
      WORD(N) = (SUM/10.0**KSAVE)*SIGN
      SUM = 0.0
      SIGN = 1.0
      DEC = 0.0
      GO TO 20
      END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR PLOT,PLOT
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4614B
THIS COMPILATION WAS DONE ON 02 MAY 68 AT 10:19:13.

      SUBROUTINE PLOT      ENTRY POINT 000510

*DIAGNOSTIC* THE NAME OR APPEARS IN A DIMENSION OR TYPE STATEMENT BUT IS NEVER REFERENCED.
    1.        SUBROUTINE PLOT(X,Y,N,N1,N2,NOUT)                                  PLOT0010
    2.        DIMENSION X(1),Y(1),IP(150),B(6),A(18),NB(6),NA(18)                PLOT0020
    3.        DIMENSION B1(6),B2(6),B3(6),NB1(6),NB2(6),NB3(6)                   PLOT0030
    4.        EQUIVALENCE (A,NA),(B,NB),(C,NC),(D,ND)                            PLOT0040
    5.        EQUIVALENCE (B1,NB1),(B2,NB2),(B3,NB3)                             PLOT0050
    6.    C   X=ABCISSA VALUES TO BE PLOTTED                                     PLOT0060
    7.    C   Y=ORDINATE VALUES TO BE PLOTTED                                    PLOT0070
    8.    C   N=NUMBER OF POINTS TO BE PLOTTED (150 OR LESS)                     PLOT0080
    9.    C   IF N IS NEGATIVE THE Y ARRAY IS IN DESCENDING ORDER                PLOT0090
   10.    C   N1=NUMBER OF PRINT WHEELS TO BE USED (108 OR LESS)                 PLOT0100
   11.    C   N2=NUMBER OF LINES TO BE USED (RECOMMEND 50)                       PLOT0110
   12.    C   NOUT=TAPE NO. OF OUTPUT TAPE                                      PLOT0120
   13.    C   RESTORATION AND HEADING OF PAGE IS LEFT TO USER                    PLOT0130
   14.    C-------------------------------------------------------------------PLOT0140
   15.    C   ALL BLANKS                                                        PLOT0150
   16.        DATA C/6H      /                                                  PLOT0160
   17.    C   ALL NEGATIVE SIGNS - BOTTOM LINE USE                             PLOT0170
   18.        DATA D/6H------/                                                   PLOT0180
   19.    C   STARS IN VARIOUS POSITIONS - BLANKS FILLED IN (6)                 PLOT0190
   20.    C   SUBSTITUTE OCTAL EQUIVALENT OF * IN THIS STATEMENT               PLOT0200
   21.        DATA B/6H<@@@@@,6H@<@@@@,6H@@<@@@,6H@@@<@@,6H@@@@<@,6H@@@@@</    PLOT0210
```

```
      C     MASK FOR PICKING OUT SECTOR                                      PLOT0220
            DATA B1/07700000000000,00077000000000,00000770000000,           PLOT0230
           10000000770000,00000000077000,00000000000770/                    PLOT0240
      C     MASK FOR COMPARING TO BLANK                                      PLOT0250
            DATA B2/6H @@@@@,6H@ @@@@,6H@@ @@@,6H@@@ @@,6H@@@@ @,6H@@@@@ /  PLOT0260
      C     MASK FOR SUBTRACTING ONE                                         PLOT0270
            DATA B3/6H[@@@@@,6H@[@@@@,6H@@[@@@,6H@@@[@@,6H@@@@[@,6H@@@@@[/  PLOT0280
           DATA LARGE/0001000000000/                                         PLOT0290
           INTEGER AND,OR                                                    PLOT0300
      C-----------------------------------------------------------------------PLOT0310
            IFLG=1                                                           PLOT0320
            IF(N.LT.0)IFLG=2                                                 PLOT0330
            N=IABS(N)                                                        PLOT0340
      C     INITIALIZES FORMAT                                               PLOT0350
            DO 9 L=1,18                                                      PLOT0360
          9 A(L)=C                                                           PLOT0370
      C     SEARCHES X POINTS FOR HIGHEST AND LOWEST VALUES                  PLOT0380
            XMIN=1.E+38                                                      PLOT0390
            XMAX=-1.E+38                                                     PLOT0400
            DO 10 I=1,N                                                      PLOT0410
            XMAX=AMAX1(XMAX,X(I))                                            PLOT0420
         10 XMIN=AMIN1(XMIN,X(I))                                            PLOT0430
            DELTAX=(XMAX-XMIN)/(FLOAT(N1-1))                                 PLOT0440
      C     REORDERS Y INTO DESCENDING VALUES                                PLOT0450
            GO TO (20,15),IFLG                                               PLOT0460
```

```
47.      15 DO 16 I=1,N                                                    PLOT0470
48.         IP(I)=I                                                        PLOT0480
49.      16 CONTINUE                                                       PLOT0490
50.         YMAX=Y(1)                                                      PLOT0500
51.         YMIN=Y(N)                                                      PLOT0510
52.         GO TO 25                                                       PLOT0520
53.      20 DO 21 I=1,N                                                    PLOT0530
54.         IP(I)=0                                                        PLOT0540
55.      21 CONTINUE                                                       PLOT0550
56.         DO 23 I=1,N                                                    PLOT0560
57.         YMAX=-1.E38                                                    PLOT0570
58.         DO 22 J=1,N                                                    PLOT0580
59.         IF(IP(J).GE.LARGE) GO TO 22                                    PLOT0590
*DIAGNOSTIC*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
60.         IF(Y(J).LE.YMAX) GO TO 22                                      PLOT0600
61.         YMAX=Y(J)                                                      PLOT0610
62.         KK=J                                                           PLOT0620
63.      22 CONTINUE                                                       PLOT0630
64.         IP(I)=IP(I)+KK                                                 PLOT0640
65.         IP(KK)=IP(KK)+LARGE                                            PLOT0650
66.      23 CONTINUE                                                       PLOT0660
67.         DO 24 I=1,N                                                    PLOT0670
68.         IP(I)=IP(I)-LARGE                                              PLOT0680
69.      24 CONTINUE                                                       PLOT0690
70.         IX1=IP(1)                                                      PLOT0700
71.         IX2=IP(N)                                                      PLOT0710
```

```
      YMAX=Y(IX1)                                                       PLOT0720
      YMIN=Y(IX2)                                                       PLOT0730
   25 DELTAY=(YMAX-YMIN)/(FLOAT(N2-1))                                  PLOT0740
      DELT=YMAX                                                         PLOT0750
C     PLOTTING SECTION                                                  PLOT0760
      DO 41 K=1,N                                                       PLOT0770
      I=IP(K)                                                           PLOT0780
      J=IP(K+1)                                                         PLOT0790
      IF(K-1)33,33,30                                                   PLOT0800
   30 IF(L)31,31,33                                                     PLOT0810
   31 DELT=DELT-DELTAY                                                  PLOT0820
      IF(Y(I)-DELT+.0001) 32, 33, 33
C     PRINTS BLANK LINES                                                PLOT0840
   32 L=-1                                                              PLOT0850
      GO TO 37                                                          PLOT0860
C     PRINT WHEEL POSITION (0,1,2,3....N1-1)                            PLOT0870
   33 NPWP=(X(I)-XMIN)/DELTAX                                           PLOT0880
C     SECTOR(1,2,3,4,5....N1/6+1)                                       PLOT0890
      NSECT=(NPWP/6)+1                                                  PLOT0900
C     POSITION IN SECTOR(1,2,3,4,5,6)                                   PLOT0910
      NF=MOD(NPWP,6)+1                                                  PLOT0920
C     PLACES * IN FORMAT                                                PLOT0930
C-----------------------------------------------------------------------PLOT0940
      NTST=AND(NA(NSECT),NB1(NF))                                       PLOT0950
      IF(NTST.EQ.NB2(NF)   )GO TO 100                                   PLOT0960
      NA(NSECT)=NA(NSECT)-NB3(NF)                                       PLOT0970
```

```
      GO TO 101                                                          PLOT0980
  100 NA(NSECT)=NA(NSECT)+NB(NF)                                         PLOT0990
  101 CONTINUE                                                           PLOT1000
C-----------------------------------------------------------------------PLOT1010
      IF(K-N)34,36,36                                                    PLOT1020
C     REPEATS IF Y(I) AND Y(J) ARE CLOSER THAN DELTAY                    PLOT1030
   34 IF(Y(J)-DELT+.0001) 36, 35, 35
   35 L=1                                                                PLOT1050
      GO TO 41                                                           PLOT1060
   36 L=0                                                                PLOT1070
C     PRINTING ROUTINE                                                   PLOT1080
   37 CONTINUE                                                           PLOT1090
      WRITE (NOUT,38)DELT,(A(IL),IL=1,18)                                PLOT1100
   38 FORMAT ( 1PE10.3, 2H I, 18A6 )
      IF(L)31,39,39                                                      PLOT1120
C     RESTORES FORMAT                                                    PLOT1130
   39 DO 40 IL=1,18                                                      PLOT1140
   40 A(IL)=C                                                            PLOT1150
   41 CONTINUE                                                           PLOT1160
C     DRAWS BOTTOM AXIS                                                  PLOT1170
      DO 42 I=1,18                                                       PLOT1180
   42 A(I)=D                                                             PLOT1190
      WRITE (NOUT,43)(A(I),I=1,18)                                       PLOT1200
   43 FORMAT(12X,18A6)                                                   PLOT1210
C     RESTORES A ARRAY TO BLANKS                                         PLOT1220
      DO 44 I=1,18                                                       PLOT1230
```

```
124.       44 A(I)=C                                                    PLOT1240
125.    C     SETS UP * EVERY 10 PLACES FOR LOWER AXIS                  PLOT1250
126.          DO 45 I=2,12,5                                            PLOT1260
127.          NA(I)=NA(I)+NB(4)                                         PLOT1270
128.          NA(I+2)=NA(I+2)+NB(2)                                     PLOT1280
129.       45 NA(I+3)=NA(I+3)+NB(6)                                     PLOT1290
130.          NA(17)=NA(17)+NB(4)                                       PLOT1300
131.          NA(1)=NA(1)+NB(1)                                         PLOT1310
132.          WRITE (NOUT,43)(A(I),I=1,18)                              PLOT1320
133.          DELTAX=((XMAX-XMIN)/FLOAT(N1))*10.0                       PLOT1330
134.          DO 46 I=1,11                                              PLOT1340
135.       46 A(I)=XMIN+FLOAT(I-1)*DELTAX                               PLOT1350
136.          WRITE (NOUT,47)(A(I),I=2,11)                              PLOT1360
137.       47 FORMAT(16X,1P10E10.4)                                     PLOT1370
138.          RETURN                                                    PLOT1380
139.          END                                                       PLOT1390
END OF LISTING.     2 *DIAGNOSTIC* MESSAGE(S).
```

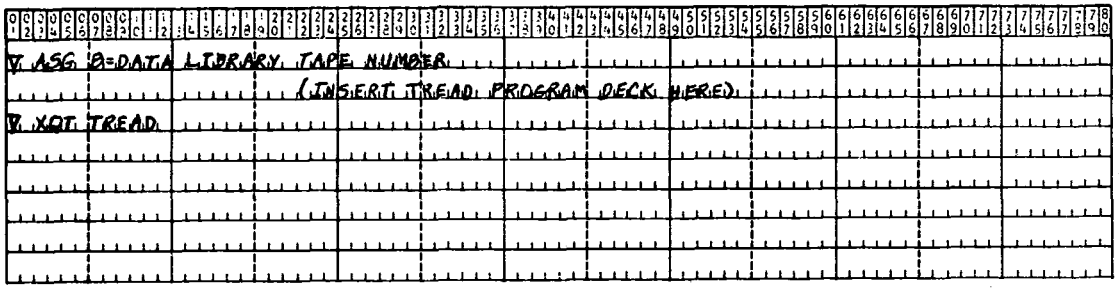
STEP 3: TREAD

This program lists the contents of the data library tape as follows:

1. All the data on the TEDIT card except column 80
2. The cycle numbers in sequence for each experiment (data section) and the number of data blocks (points) that are in each cycle

A version of this program called TREAD LONG PRINT lists signal + noise, noise, and current values for each channel number.

Below is a typical TREAD deck setup.




A program listing follows.

```
@ FOR TREAD,TREAD
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 02 MAY 68 AT 10:19:05

   MAIN PROGRAM          ENTRY POINT 000000

 1.    C.. THE PURPOSE OF THIS ROUTINE IS TO READ THE LIBRARY TAPE AND LIST ALL
 2.    C    DATA BY RUN NUMBER AND BY CYCLE NUMBER.
 3.          INTEGER CHAN
 4.          REAL NOISE
 5.          DIMENSION CHAN(100), SPLUSN(100), NOISE(100), CURR(100), DATE(2)
 6.          PARAMETER LTAPE = 10
 7.          REWIND LTAPE
 8.        8 READ(LTAPE) NUM, ITYPE, VAR, TIME, RES, DVOLT, VOLTST, TINT,
 9.         1 SIGMIN, SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
10.          WRITE(6,11) NUM
11.       11 FORMAT( 10X, 10HRUN NUMBER, 1X, A6, /  )
12.          WRITE(6,12) ITYPE
13.       12 FORMAT( 10X, 3HGAS, 1X, A6, / )
14.          WRITE(6,13) VAR
15.       13 FORMAT( 10X, 10HVARIANCE %, 1X, F6.2, / )
16.          WRITE(6,14) TIME
17.       14 FORMAT( 10X, 4HTIME, 1X, A6, / )
18.          WRITE(6,15) RES
19.       15 FORMAT( 10X, 4HRES. 1X, F6.2, / )
20.          WRITE(6,16) DVOLT
21.       16 FORMAT( 10X, 17HVOLTAGE INCREMENT, 1X, F6.2, / )
22.          WRITE(6,17) VOLTST
```

```
      17 FORMAT( 10X, 17HSTARTING VOLTAGE , 1X, F6.2, / )
         WRITE(6,18) TINT
      18 FORMAT( 10X, 14HTIME INTERVAL , F6.2, / )
         WRITE(6,19) SIGMIN
      19 FORMAT( 10X, 12HMIN. SIGNAL , F10.2, / )
         WRITE(6,20) SIGMAX
      20 FORMAT( 10X, 12HMAX. SIGNAL , F10.2, / )
         WRITE(6,21) CURMIN
      21 FORMAT( 10X, 13HMIN. CURRENT , F10.2, / )
         WRITE(6,22) CURMAX
      22 FORMAT( 10X, 13HMAX. CURRENT , F10.2, / )
         WRITE(6,23) DATE(1), DATE(2)
      23 FORMAT( 10X,  4HDATE, 1X, 2A6, / )
      10 READ(LTAPE) KOUNT, L
C
         WRITE(6,24) KOUNT
      24 FORMAT( 1H1, 10X, 12HCYCLE NUMBER, 1X, I3, / )                    L. PRNT
         WRITE(6,25) L
      25 FORMAT( 10X, 16HNUMBER OF POINTS, I5, //  )
C
         READ(LTAPE) (CHAN(I), SPLUSN(I), NOISE(I), CURR(I), I=1,L )
         WRITE(6,27) (CHAN(I), SPLUSN(I), NOISE(I), CURR(I), I=1,L )       L. PRNT
      27 FORMAT( I10, 3F10.1 )                                             L. PRNT
         READ(LTAPE) LAST
         IF(LAST.EQ.0) GO TO 10
         WRITE(6,31)
```

```
   49.      31 FORMAT( 1H1 )
   50.         IF(LAST.EQ.1) GO TO 8
   51.         WRITE(6,28)
   52.      28 FORMAT(/ 12H END OF FILE )
   53.         CALL REWI(LTAPE)
   54.         CALL EXIT
   55.         END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

STEP 4: ABEAM4

Input for this program consists of the data library tape, as written by TEDIT, and a set of data cards. The purpose of the program is to perform various calculations based on data from different cycles of the same experiment or from different experiments.

The normal output from ABEAM4 is the following (see option 3, below):

1. Σ signal
2. Σ signal smoothed once
3. Σ (signal + noise)
4. Σ (signal + noise) smoothed once
5. Σ (signal/noise)
6. Σ noise
7. Σ current

Printer plots of the following are also given:

1. Σ signal
2. Σ signal smoothed once
3. Σ (signal + noise)
4. Σ (signal + noise) smoothed once
5. Σ (signal/noise)
6. Σ noise

By the use of an option (see option 1, below), the additional information may be obtained along with a printer plot of each.

1. first derivative of Σ signal
2. first derivative of Σ signal smoothed once
3. first derivative of Σ signal smoothed twice
4. second derivative of Σ signal smoothed twice
5. first derivative of Σ (signal + noise) smoothed once

The input card formats are as follows:

Title Card: FORTRAN format is (12A6)

| Column | |
|---|---|
| 1-72 | Title (printed at top of first page) |

Option Card: FORTRAN format is (3I6)

| Column | |
|---|---|
| 6 | Option 1 = 0 or blank: derivative output not desired<br>= 1: desire derivative output |
| 12 | Option 2 = 0 or blank: parabolic least squares fit for smoothing<br>= 1: Fourier series smoothing |
| 18 | Option 3 = 0 or blank: all output is calculated as shown below<br>= 1: each term in the summation is divided by its respective value of current (i. e., Σ (signal/current) etc.) |

Run No. Card: FORTRAN format is (A6, 2I6)

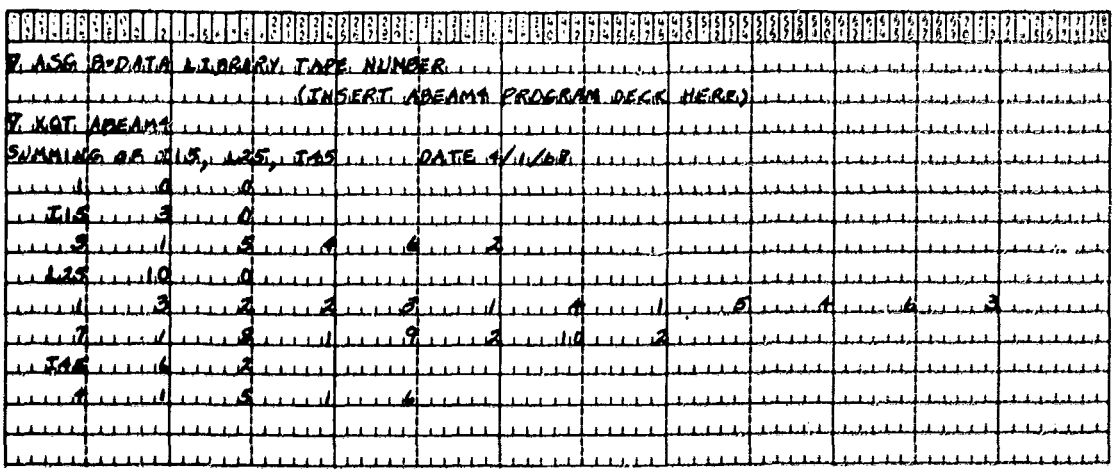
| Column | |
|---|---|
| 1-6 | Experiment number (IRUN) |
| 7-12 | Number of cycles (NCYC) requested from this experiment |
| 18 | ILAST = 0 or blank: another Run No. card follows the Cycle No. card<br>= 1: another title card follows the next Cycle No. card<br>= 2: no more cards follow the next Cycle No. card. The next Cycle No. card is the last to be summed and all processing is complete |

Cycle No. Card: FORTRAN format is (12I6)

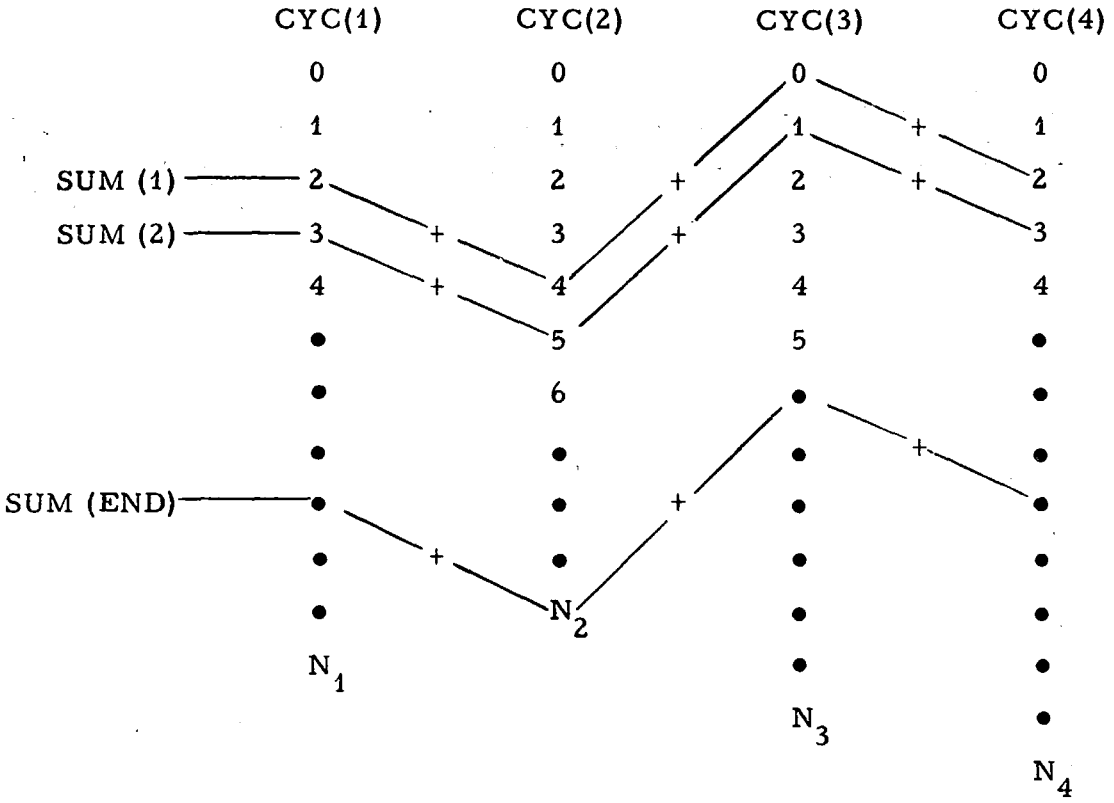
| Column | |
|---|---|
| 1-6 | Cyc (1) = first requested cycle number |
| 7-12 | REFPNT (1) |
| 13-18 | Cyc (2) = second requested cycle number |
| 19-24 | REFPNT (2) |
| . | . |
| . | . |
| . | . |
| 25-66 | Cyc (6) = sixth requested cycle number |
| 67-72 | REFPNT (6) |

Two or more cards of this type may be used if the number of cycles (NCYC) requested exceeds six.

Below is an example deck setup for summing together cycles 3, 5, and 6 from experiment I15; cycles 1 through 10 of experiment L25; and cycles 4 through 9 from experiment I45.




Below is a diagram showing how the summing, $\Sigma$, takes place with reference to the channel numbers.




In the diagram, CYC(1) through CYC(4) are arbitrary cycles. The reference points, REFPNT(1) through REFPNT(4), are 3, 5, 1, 3, respectively. In this particular case $N_2 < N_1 < N_3 < N_4$; therefore, it is meaningless to sum past $N_2$. The total number of sums that would be printed is $(N_2 - 4) + 1$.

A program listing follows.

```
GP FOR ABEAM4,ABEAM4
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 29 MAY 68 AT 13:59:52

   MAIN PROGRAM          ENTRY POINT 000000

 1.          PARAMETER LTAPE = 10
 2.          PARAMETER ID=200
 3.          INTEGER PCHAR, SLI
 4.          INTEGER BLANK, CYC, REFPNT, OPT1, OPT2, OPT3, RFPNT1, OPT4
 5.          REAL NOISE
 6.          DIMENSION SPLUSN(100), NOISE(100), SIG(100), SIG1(100), SIG2(100),
 7.         1  SPN(100), SPN1(100), SIGDN(100), DSPN1(100), DSIG(100), IP(100),
 8.         2  DSIG1(100), DSIG2(100), D2SIG2(100), NUMTAB(ID), TITLE(12),
 9.         3 CYC(ID), REFPNT(ID), CURR(100), SNOISE(100), VOLT(100),
10.         4 SUMCUR(100)
11.          DATA BLANK/6H      /,SLI/2H/I/
12.          COMMON DVOLT, KEY
13.          REWIND LTAPE
14.          DO 5 I=1,ID
15.        5 NUMTAB(I) = 0
16.       10 IGB = 1
17.          IGE = 100
18.          ITIME = 0
19.          ILAST = 0
20.          READ(5,11) (TITLE(I), I=1,12)
```

```
      11 FORMAT( 12A6)
         WRITE(6,13) (TITLE(I), I=1,12)
      13 FORMAT( 1H1, 30X, 12A6, // 40X 32HREQUESTED DATA FROM LIBRARY TAPE
     1   )
         DO 14 I=1,100
         SPN(I) = 0.0
         SIG(I) = 0
         SIGDN(I) = 0
         SUMCUR(I) = 0.0
      14 SNOISE(I) = 0.0
         READ(5,15) OPT1, OPT2, OPT3, OPT4
      15 FORMAT( 12I6 )
      16 IF(ILAST) 150, 20, 150
      20 READ(5,21) IRUN, NCYC, ILAST
      21 FORMAT( A6, 11I6 )
         READ(5,22) (CYC(I), REFPNT(I), I=1,NCYC )
      22 FORMAT( 12I6 )
         WRITE(6,24) (IRUN, CYC(I), REFPNT(I), I=1,NCYC)
      24 FORMAT( /  40X, 4HRUN , A6, 2X, 5HCYCLE, I3, 2X, 10HREF. POINT I3)
         IF(ITIME.NE.0) GO TO 28
         REFPNT1 = REFPNT(1)
         IGB = REFPNT(1)
         ITIME = 1
C.. CHECK RUN NUMBER TABLE TO SEE TAPE DATA CAN BE FOUND BY FORWARD READING.
      28 DO 30 I=1,ID
         IF(IRUN.EQ.NUMTAB(I) ) GO TO 40
         IF(NUMTAB(I).NE.0) GO TO 30
```

```
      IPOS = I - 1
      GO TO 50
   30 CONTINUE
   40 REWIND LTAPE
      DO 45 I=1,ID
   45 NUMTAB(I) = 0
      IPOS = 0
   50 READ(LTAPE) NUM, DUMMY, DUMMY,DUMMY, DUMMY, DVOLT, VOLTST
      IPOS = IPOS + 1
      NUMTAB(IPOS) = NUM
      IF(NUM.EQ.IRUN) GO TO 70
C.. POSITION TAPE TO READ NEXT RUN NUMBER ON TAPE.
   55 READ(LTAPE) DUMMY, L
      READ(LTAPE) (DUMMY, DUMMY, DUMMY, DUMMY, I=1,L )
      READ(LTAPE) LAST
      IF(LAST-1) 55, 50, 60
   60 WRITE(6,61) IRUN
   61 FORMAT(   4H RUN A6, 28H IS NOT ON THE LIBRARY TAPE. )
      CALL REWI(LTAPE)
      CALL EXIT
C.. REQUESTED RUN HAS BEEN FOUND. PICK OUT REQUESTED CYCLES.
   70 DO 140 J=1,NCYC
   72 READ(LTAPE) ICYC, L
      READ(LTAPE) ( DUMMY, SPLUSN(I), NOISE(I), CURR(I), I=1,L )
      READ(LTAPE) LAST
      IF(ICYC.NE.CYC(J)) GO TO 130
C.. CALC. BEGINNING AND ENDING SUBCRIPTS BASED UPON REF. POINT NUMBER.
```

```
      NDIF = REFPNT(J) - RFPNT1
      IF(NDIF) 80, 90, 100
   80 IGB = MAX0(IGB,1-NDIF)
      IGE = MIN0(IGE,IGB+(L-REFPNT(J)) )
      GO TO 110
   90 IGB = IGB
      IGE = MIN0(IGE,L)
      GO TO 110
  100 IGB = IGB
      IGE = MIN0(IGE,L-NDIF)
  110 DO 120 I=IGB,IGE
      NA = I + NDIF
      D = 1.0
      IF(OPT3.NE.0) D = CURR(NA)
      SPN(I) = SPN(I) + SPLUSN(NA)/D
      SIG(I) = SIG(I) + (SPLUSN(NA)-NOISE(NA))/D
      SNOISE(I) = SNOISE(I) + NOISE(NA)/D
      SIGDN(I) = SIGDN(I) + (SPLUSN(NA)-NOISE(NA))/(NOISE(NA)*D)
      SUMCUR(I) = SUMCUR(I) + CURR(NA)
  120 CONTINUE
      GO TO 140
  130 IF(LAST.EQ.0) GO TO 72
      WRITE(6,131) CYC(J)
  131 FORMAT(  13H CYCLE NUMBER I6,28H IS NOT ON THE LIBRARY TAPE. )
      CALL REWI (LTAPE)
      CALL EXIT
  140 CONTINUE
```

```
C.. POSITION TAPE AT THE BEGINNING OF THE NEXT LOGICAL RECORD CONTAINING
C   THE NEXT RUN NUMBER.
C
C.. CHECK FOR END OF FILE FIRST.
  142 IF(LAST.NE.2) GO TO 146
      REWIND LTAPE
      DO 144 I=1,ID
  144 NUMTAB(I) = 0
      GO TO 16
C.. IF LAST EQUALS ONE TAPE IS POSITION ALREADY.
  146 IF(LAST.EQ.1) GO TO 16
C.. THERE STILL REMAINS SOME CYCLES.
      READ(LTAPE) DUMMY, L
      READ(LTAPE) (DUMMY, DUMMY, DUMMY, DUMMY, I=1,L)
      READ(LTAPE) LAST
      GO TO 142
C
  150 X = 0
      DO 160 I=IGB,IGE
      X = X + 1
  160 VOLT(I) = VOLTST + (X-1.0)*DVOLT
C.. RE-ORDER ARRAYS
      IGBM1 = IGB - 1
      DO 162 I=IGB,IGE
      IA = I - IGBM1
      SIG(IA) = SIG(I)
      SPN(IA) = SPN(I)
```

```
      SNOISE(IA) = SNOISE(I)
      SIGDN(IA) = SIGDN(I)
      VOLT(IA) = VOLT(I)
      IP(IA) = I
      SUMCUR(IA) = SUMCUR(I)
  162 CONTINUE
      NUMPTS = IGE - IGBM1
      KEY = 1
      CALL SMT (SIG, SIG1, NUMPTS, OPT2)
      KEY = 2
      CALL SMT (SPN, SPN1, NUMPTS, OPT2)
      IF( OPT3.EQ.0) GO TO 169
      WRITE(6,168)
  168 FORMAT( 1H1, 12X 5HVOLTS 11X 3HS/I 12X 3HS/I 2X 2(8X 7H(S+N)/I),
     *  6X  11H  S/(N*I)  , 8X 3HN/I  13X 1HI )
      GO TO 1711
  169 WRITE(6,170)
  170 FORMAT( 1H1, 12X 5HVOLTS 12X 1HS 14X 1HS 1X 2(12X 3HS+N), 12X
     *  3HS/N 13X 1HN 14X 1HI )
 1711 WRITE(6,171)
  171 FORMAT( 20X  2(22X, 8H(SMTH 1) )  /  )
      WRITE(6,172) ( IP(I), VOLT(I), SIG(I), SIG1(I), SPN(I), SPN1(I),
     1 SIGDN(I), SNOISE(I), SUMCUR(I), I=1,NUMPTS )
  172 FORMAT( 3X, 13, 1P8E15.6 )
C.. PLOT ABOVE ITEMS ON PRINTER.
      PCHAR = BLANK
      IF( OPT3.NE.0) PCHAR = SLI
```

```
      WRITE(6,173) PCHAR
  173 FORMAT( 1H1, 20X 9HPLOT OF S, A2 )
      CALL PLOT ( VOLT, SIG, NUMPTS, 100, 46, 6 )
      WRITE(6,174) PCHAR
  174 FORMAT( 1H1, 20X 9HPLOT OF S, A2, 5X 13HSMOOTHED ONCE )
      CALL PLOT ( VOLT, SIG1, NUMPTS, 100, 46, 6 )
      WRITE(6,175) PCHAR
  175 FORMAT( 1H1, 20X 13HPLOT OF (S+N), A2  )
      CALL PLOT (  VOLT, SPN, NUMPTS, 100, 46, 6 )
      WRITE(6,176) PCHAR
  176 FORMAT( 1H1, 20X 13HPLOT OF (S+N), A2, 5X 13HSMOOTHED ONCE )
      CALL PLOT (  VOLT, SPN1, NUMPTS, 100, 46, 6 )
      IF(OPT3.EQ.0) GO TO 1770
      WRITE(6,1761)
 1761 FORMAT( 1H1, 20X, 15HPLOT OF S/(N*I)  )
      GO TO 178
 1770 WRITE(6,177)
  177 FORMAT( 1H1, 20X, 11HPLOT OF S/N       )
  178 CALL PLOT ( VOLT, SIGDN, NUMPTS, 100, 46, 6 )
      WRITE(6,179) PCHAR
  179 FORMAT( 1H1, 20X, 9HPLOT OF N, A2  )
      CALL PLOT (VOLT, SNOISE, NUMPTS, 100, 46, 6 )
      IF(OPT1.EQ.0) GO TO 260
      CALL DIFF( SIG, DSIG, NUMPTS )
      CALL DIFF( SIG1, DSIG1, NUMPTS )
      KEY = 3
      CALL SMT (SIG1, SIG2, NUMPTS, OPT2)
```

```
      CALL DIFF( SIG2, DSIG2, NUMPTS )
      CALL DIFF ( DSIG2, D2SIG2, NUMPTS )
      CALL DIFF ( SPN1, DSPN1, NUMPTS )
      DXINV = 1./DVOLT
      DO 180 I=1,NUMPTS
      DSIG(I) = DSIG(I)*DXINV
      DSIG1(I) = DSIG1(I)*DXINV
      DSIG2(I) = DSIG2(I)*DXINV
      D2SIG2(I) = D2SIG2(I)*DXINV*DXINV
  180 DSPN1(I) = DSPN1(I)*DXINV
C
  190 WRITE(6,191) PCHAR, PCHAR, PCHAR, PCHAR, PCHAR
  191 FORMAT( 1H1, 12X 5HVOLTS 10X 3( 8H1ST DER., 7X), 8H2ND DER.  ,
     1 7X 8H1ST DER. / 29X 2H S, A2, 7X 2H S, A2, 7H SMTH 1, 2(4X, 2H S,
     2 A2, 7H SMTH 2  ), 4X 5H(S+N), A2, 7H SMTH 1 / )
  200 WRITE(6,201) (IP(I), VOLT(I), DSIG(I), DSIG1(I), DSIG2(I),
     1  D2SIG2(I), DSPN1(I), I=1,NUMPTS )
  201 FORMAT( 3X, I3, 1P6E15.6 )
C.. PLOT ABOVE ITEMS ON PRINTER.
      WRITE(6,211) PCHAR
  211 FORMAT( 1H1, 20X 15HDERIVATIVE OF S, A2 )
      CALL PLOT ( VOLT, DSIG, NUMPTS, 100, 46, 6 )
      WRITE(6,221) PCHAR
  221 FORMAT( 1H1, 20X 15HDERIVATIVE OF S, A2,14H SMOOTHED ONCE )
      CALL PLOT ( VOLT, DSIG1, NUMPTS, 100, 46, 6 )
      WRITE(6,231) PCHAR
  231 FORMAT( 1H1, 20X,  15HDERIVATIVE OF S, A2, 15H SMOOTHED TWICE )
```

```
      CALL PLOT ( VOLT, DSIG2, NUMPTS, 100, 46, 6 )
      WRITE(6,241) PCHAR
  241 FORMAT( 1H1, 20X,19H2ND DERIVATIVE OF S, A2, 15H SMOOTHED TWICE )
      CALL PLOT ( VOLT, D2SIG2, NUMPTS, 100, 46, 6 )
      WRITE(6,251) PCHAR
  251 FORMAT( 1H1, 20X,19HDERIVATIVE OF (S+N), A2, 14H SMOOTHED ONCE  )
      CALL PLOT ( VOLT, DSPN1, NUMPTS, 100, 46, 6 )
C
  260 IF(OPT4.EQ.0) GO TO 280
      DO 270 J=1,3
      PUNCH 261, (TITLE(I),I=1,12)
  261 FORMAT(12A6)
      PUNCH 262,
  262 FORMAT( 5X, 1H0, 5X, 1H0 )
      PUNCH 263, VOLT(1), VOLT(NUMPTS), DVOLT
  263 FORMAT( 3F12.4)
      GO TO (264, 265, 266), J
  264 PUNCH 267, (SIG(I), I=1,NUMPTS)
      GO TO 270
  265 PUNCH 267, (SPN(I), I=1,NUMPTS)
      GO TO 270
  266 PUNCH 267, (SNOISE(I), I=1,NUMPTS)
  267 FORMAT( 6F12.4 )
  270 CONTINUE
  280 IF(ILAST.EQ.1) GO TO 10
      CALL REWI ( LTAPE )
      CALL EXIT
```

```
237.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR SMT,SMT
UNIVAC 1106 FORTRAN IV LEVEL  2201 0029 F46148
THIS COMPILATION WAS DONE ON 01 MAY 68 AT 14:22:13

   SUBROUTINE SMT       ENTRY POINT 000471

 1.         SUBROUTINE SMT ( Y, YC, NP, IOPT )
 2.   C     ROUTINE TO SMOOTH CURVE                                          SMT  030
 3.         DIMENSION Y(1), YC(1), B(100)
 4.         COMMON DX, KEY
 5.         PI = 3.1415926
 6.         IF(IOPT.GT.0) GO TO 200
 7.         NPM1 = NP - 1
 8.         NPM2 = NP - 2
 9.         DO 100 I=3,NPM2                                                  SMT  050
10.         YC(I)=Y(I)-8.5714286E-02*(Y(I-2)-4.0*(Y(I-1)+Y(I+1))+6.0*Y(I)+Y(I+SMT  060
11.        12))                                                             SMT  070
12.    100 CONTINUE                                                         SMT  080
13.         YC(1)=Y(1)                                                       SMT  090
14.         YC(2)=0.25*(Y(1)+2.0*Y(2)+Y(3))                                  SMT  100
15.         YC(NPM1)=0.25*(Y(NPM2)+2.0*Y(NPM1)+Y(NP))                        SMT  110
16.         YC(NP)=Y(NP)                                                     SMT  120
17.         RETURN                                                           SMT  130
18.    200 P = NP-1
19.         HL = P*DX
20.         YMIN = 1.E+37
21.         DO 205 I=1,NP
22.         YMIN = AMIN1(YMIN,Y(I))
```

```
205 CONTINUE
    IF(YMIN.LT.0) GO TO 208
    DO 206 I=1,NP
    YC(I) = Y(I)
206 CONTINUE
    GO TO 210
208 DO 209 I=1,NP
    YC(I) = Y(I) - YMIN
209 CONTINUE
210 YI = SQRT( YC(1) )
    YF = (SQRT( YC(NP) ) - YI)/HL
    X = 0
    DO 211 I=1,NP
    YC(I) = SQRT( YC(I) ) - YI - YF*X
211 X = X + DX
    CALL FOUR (NP, YC, B )
    NPM = NP-1
    GO TO (212, 214, 216), KEY
212 WRITE(6,213)
213 FORMAT( 1H1, 20X 46HFOURIER COEFFICIENTS FOR SMOOTHING SIGNAL ANCE
   * )
    GO TO 218
214 WRITE(6,215)
215 FORMAT( 1H1, 20X 54HFOURIER COEFFICIENTS FOR SMOOTHING SIGNAL + NO
   *ISE ONCE )
```

```
      GO TO 218
  216 WRITE(6,217)
  217 FORMAT( 1H1, 20X 47HFOURIER COEFFICIENTS FOR SMOOTHING SIGNAL TWIC
     *E )
  218 WRITE(6,219) (B(I), I=1,NPM )
  219 FORMAT( 10X  10E10.3 )
      DO 220 I=1,NPM
      CI = I
  220 B(I) = B(I)*COS(PI*CI/(2.0*P))**2
      WRITE(6,221)
  221 FORMAT( /  20X,  40HFOURIER COEFFICIENTS FILTERED BY COS**2  )
      WRITE(6,219) (B(I), I=1,NPM )
      IF(IOPT.EQ.1) GO TO 230
      NMAX = IOPT
      GO TO 300
  230 BT = 0.0
      DO 240 I=1,20
      NPI = NP-1
  240 BT = BT+B(NPI)**2
      K = 20
  245 N = NP-K
      BE = B(N-1)**2
      CK = K
      BET = BT/CK
      IF(BE/BET-16.0) 250,250, 280
```

```
      250 IF(N-2) 260, 260, 270
      260 NMAX = NP/10
          WRITE(6,261)
      261 FORMAT( 20X, 11HTEST FAILED )
          GO TO 300
      270 K = K+1
          BT = BT + BE
          GO TO 245
      280 IF(N-25) 290, 270, 270
      290 NMAX = N+2
      300 WRITE(6,301) NMAX
      301 FORMAT( / 20X, 22HSMOOTHING ROUTINE USED I3,13H COEFFICIENTS )
          CALL FOURI ( NMAX, NP, B, YC )
          X = 0
          DO 310 K=1,NP
          YK = YC(K) + YI + YF*X
          YC(K) = YK*YK
      310 X = X + DX
          IF(YMIN.LT.0) GO TO 320
          RETURN
      320 DO 330 I=1,NP
          YC(I) = YC(I) + YMIN
      330 CONTINUE
          RETURN
          END                                                    CMT 140
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOUR,FOUR
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 01 MAY 68 AT 14:22:16

   SUBROUTINE FOUR      ENTRY POINT 000127
 1.          SUBROUTINE FOUR(NP,Y,B)
 2.          DIMENSION Y(1), B(1)
 3.          PI = 3.141592653
 4.          CNP = NP
 5.          NPM = NP-1
 6.          CNPM = NPM
 7.          PION = PI/CNPM
 8.          COSZ = COS(PION)
 9.          SINZ = SIN(PION)
10.          COSK = COSZ
11.          SINK = SINZ
12.          DO 20 K =1,NPM
13.          BK = 0.0
14.          COSKI = COSK
15.          SINKI = SINK
16.          DO 22 I = 2,NPM
17.          BK = BK + Y(I)*SINKI
18.          SINI = SINKI*COSK+COSKI*SINK
19.          COSI = COSKI*COSK-SINKI*SINK
20.          SINKI = SINI
21.       22 COSKI = COSI
22.          SINKI = SINK*COSZ+COSK*SINZ
```

```
      COSKI = COSK*COSZ-SINK*SINZ
      COSK =COSKI
      SINK =SINKI
   20 B(K)=2.0*BK/CNP
      RETURN
      END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOURI,FOURI
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 01 MAY 68 AT 14:22:17

   SUBROUTINE FOURI     ENTRY POINT 000142

 1.          SUBROUTINE FOURI ( NMAX, NP, B, Y )
 2.          DIMENSION B(1), Y(1)
 3.          NPM = NP-1
 4.          CNPM = NPM
 5.          PI = 3.141592653
 6.          PIOM = PI/CNPM
 7.          COSZ = COS(PIOM)
 8.          SINZ = SIN(PIOM)
 9.          Y(1) = 0.0
10.          COSK = COSZ
11.          SINK = SINZ
12.          DO 20 K = 2,NP
13.          YK = 0.0
14.          PIK = PIOM
15.          COSKI = COSK
16.          SINKI = SINK
17.          DO 22 I =1,NMAX
18.          YK = YK+B(I)*SINKI
19.          YDK = YDK + PIK*B(I)*COSKI
20.          PIK = PIK+PIOM
21.          SINI = SINKI*COSK+COSKI*SINK
22.          COSI = COSKI*COSK-SINKI*SINK
```

```
      COSKI = COSI
      SINKI = SINI
   22 CONTINUE
      COSKI = COSK*COSZ-SINK*SINZ
      SINKI = COSK*SINZ+SINK*COSZ
      COSK = COSKI
      SINK = SINKI
   20 Y(K) = YK
      RETURN
      END
```

END OF LISTING.  0 *DIAGNOSTIC* MESSAGE(S).

```
@P FOR DIFF,DIFF
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 01 MAY 68 AT 14:22:18

   SUBROUTINE DIFF      ENTRY POINT 000031


  1.          SUBROUTINE DIFF(Y,YD,NP)                                  DIFF 020
  2.    C     ROUTINE TO TAKE DIFFERENCES                               DIFF 030
  3.          DIMENSION  Y(1)       ,YD(1)                              DIFF 040
  4.    C                                                               DIFF 050
  5.          NPM1 = NP - 1
  6.          DO 100 I=2,NPM1                                           DIFF 060
  7.          YD(I)=(Y(I+1)-Y(I-1))*0.5                                 DIFF 070
  8.      100 CONTINUE                                                  DIFF 080
  9.          YD(1)=Y(2)-Y(1)                                           DIFF 090
 10.          YD(NP)=Y(NP)-Y(NPM1)                                      DIFF 100
 11.          RETURN                                                    DIFF 110
 12.          END                                                       DIFF 120
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@P FOR PLOT,PLOT
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 01 MAY 68 AT 14:22:20

    SUBROUTINE PLOT      ENTRY POINT 000510

*DIAGNOSTIC*  THE NAME OR APPEARS IN A DIMENSION OR TYPE STATEMENT BUT IS NEVER REFERENCED.
    1.        SUBROUTINE PLOT(X,Y,N,N1,N2,NOUT)                              PLOT0010
    2.        DIMENSION X(1),Y(1),IP(150),B(6),A(18),NB(6),NA(18)            PLOT0020
    3.        DIMENSION B1(6),B2(6),B3(6),NB1(6),NB2(6),NB3(6)               PLOT0030
    4.        EQUIVALENCE (A,NA),(B,NB),(C,NC),(D,ND)                        PLOT0040
    5.        EQUIVALENCE (B1,NB1),(B2,NB2),(B3,NB3)                         PLOT0050
    6.  C     X=ABCISSA VALUES TO BE PLOTTED                                 PLOT0060
    7.  C     Y=ORDINATE VALUES TO BE PLOTTED                                PLOT0070
    8.  C     N=NUMBER OF POINTS TO BE PLOTTED (150 OR LESS)                 PLOT0080
    9.  C     IF N IS NEGATIVE THE Y ARRAY IS IN DESCENDING ORDER            PLOT0090
   10.  C     N1=NUMBER OF PRINT WHEELS TO BE USED (108 OR LESS)             PLOT0100
   11.  C     N2=NUMBER OF LINES TO BE USED (RECOMMEND 50)                   PLOT0110
   12.  C     NOUT=TAPE NO. OF OUTPUT TAPE                                   PLOT0120
   13.  C     RESTORATION AND HEADING OF PAGE IS LEFT TO USER                PLOT0130
   14.  C-------------------------------------------------------------------PLOT0140
   15.  C     ALL BLANKS                                                     PLOT0150
   16.  C     ALL NEGATIVE SIGNS - BOTTOM LINE USE                           PLOT0170
   17.        DATA C/6H      /                                               PLOT0160
   18.        DATA D/6H------/                                               PLOT0180
   19.  C     STARS IN VARIOUS POSITIONS - BLANKS FILLED IN (6)              PLOT0190
   20.  C     SUBSTITUTE OCTAL EQUIVALENT OF * IN THIS STATEMENT             PLOT0200
```

```
      DATA B/6H<@@@@@,6H@<@@@@,6H@@<@@@,6H@@@<@@,6H@@@@<@,6H@@@@@<,
C     MASK FOR PICKING OUT SECTOR
      DATA B1/0770000000000,0007700000000,0000077000000,
     1000000770000,0000000007700,0000000000077/
C     MASK FOR COMPARING TO BLANK
      DATA B2/6H @@@@@,6H@ @@@@,6H@@ @@@,6H@@@ @@,6H@@@@ @,6H@@@@@ ,
C     MASK FOR SUBTRACTING ONE
      DATA B3/6H[@@@@@,6H@[@@@@,6H@@[@@@,6H@@@[@@,6H@@@@[@,6H@@@@@[,
      DATA LARGE/0001000000000/
      INTEGER AND,OR
C-----------------------------------------------------------------------
      IFLG=1
      IF(N.LT.0)IFLG=2
      N=IABS(N)
C     INITIALIZES FORMAT
      DO 9 L=1,18
    9 A(L)=C
C     SEARCHES X POINTS FOR HIGHEST AND LOWEST VALUES
      XMIN=1.E+38
      XMAX=-1.E+38
      DO 10 I=1,N
      XMAX=AMAX1(XMAX,X(I))
   10 XMIN=AMIN1(XMIN,X(I))
      DELTAX=(XMAX-XMIN)/(FLOAT(N1-1))
C     REORDERS Y INTO DESCENDING VALUES
```

PLOT0210
PLOT0220
PLOT0230
PLOT0240
PLOT0250
PLOT0260
PLOT0270
PLOT0280
PLOT0290
PLOT0300
PLOT0310
PLOT0320
PLOT0330
PLOT0340
PLOT0350
PLOT0360
PLOT0370
PLOT0380
PLOT0390
PLOT0400
PLOT0410
PLOT0420
PLOT0430
PLOT0440
PLOT0450

```
      GO TO (20,15),IFLG                                                PLOT0460
   15 DO 16 I=1,N                                                       PLOT0470
      IP(I)=I                                                           PLOT0480
   16 CONTINUE                                                          PLOT0490
      YMAX=Y(1)                                                         PLOT0500
      YMIN=Y(N)                                                         PLOT0510
      GO TO 25                                                          PLOT0520
   20 DO 21 I=1,N                                                       PLOT0530
      IP(I)=0                                                           PLOT0540
   21 CONTINUE                                                          PLOT0550
      DO 23 I=1,N                                                       PLOT0560
      YMAX=-1.E38                                                       PLOT0570
      DO 22 J=1,N                                                       PLOT0580
      IF(IP(J).GE.LARGE) GO TO 22                                       PLOT0590
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
      IF(Y(J).LE.YMAX) GO TO 22                                         PLOT0600
      YMAX=Y(J)                                                         PLOT0610
      KK=J                                                              PLOT0620
   22 CONTINUE                                                          PLOT0630
      IP(I)=IP(I)+KK                                                    PLOT0640
      IP(KK)=IP(KK)+LARGE                                               PLOT0650
   23 CONTINUE                                                          PLOT0660
      DO 24 I=1,N                                                       PLOT0670
      IP(I)=IP(I)-LARGE                                                 PLOT0680
   24 CONTINUE                                                          PLOT0690
```

```
      IX1=IP(1)                                                        PLOT0700
      IX2=IP(N)                                                        PLOT0710
      YMAX=Y(IX1)                                                      PLOT0720
      YMIN=Y(IX2)                                                      PLOT0730
   25 DELTAY=(YMAX-YMIN)/(FLOAT(N2-1))                                 PLOT0740
      DELT=YMAX                                                        PLOT0750
C     PLOTTING SECTION                                                 PLOT0760
      DO 41 K=1,N                                                      PLOT0770
      I=IP(K)                                                          PLOT0780
      J=IP(K+1)                                                        PLOT0790
      IF(K-1)33,33,30                                                  PLOT0800
   30 IF(L)31,31,33                                                    PLOT0810
   31 DELT=DELT-DELTAY                                                 PLOT0820
      IF(Y(I)-DELT+.001) 32, 33, 33
C     PRINTS BLANK LINES                                               PLOT0840
   32 L=-1                                                             PLOT0850
      GO TO 37                                                         PLOT0860
C     PRINT WHEEL POSITION (0,1,2,3....N1-1)                           PLOT0870
   33 NPWP=(X(I)-XMIN)/DELTAX                                          PLOT0880
C     SECTOR(1,2,3,4,5....N1/6+1)                                      PLOT0890
      NSECT=(NPWP/6)+1                                                 PLOT0900
C     POSITION IN SECTOR(1,2,3,4,5,6)                                  PLOT0910
      NF=MOD(NPWP,6)+1                                                 PLOT0920
C     PLACES * IN FORMAT                                               PLOT0930
C-----------------------------------------------------------------     PLOT0940
```

```
      NTST=AND(NA(NSECT),NB1(NF))                                        PLOT0950
      IF(NTST.EQ.NB2(NF)    )GO TO 100                                   PLOT0960
      NA(NSECT)=NA(NSECT)-NB3(NF)                                        PLOT0970
      GO TO 101                                                          PLOT0980
  100 NA(NSECT)=NA(NSECT)+NB(NF)                                         PLOT0990
  101 CONTINUE                                                           PLOT1000
C-----------------------------------------------------------------------PLOT1010
      IF(K-N)34,36,36                                                    PLOT1020
C     REPEATS IF Y(I) AND Y(J) ARE CLOSER THAN DELTAY                    PLOT1030
   34 IF(Y(J)-DELT+.001) 36, 35, 35
   35 L=1                                                                PLOT1050
      GO TO 41                                                           PLOT1060
   36 L=0                                                                PLOT1070
C     PRINTING ROUTINE                                                   PLOT1080
   37 CONTINUE                                                           PLOT1090
      WRITE (NOUT,38)DELT,(A(IL),IL=1,18)                                PLOT1100
   38 FORMAT ( 1PE10.3, 2H I, 18A6 )
      IF(L)31,39,39                                                      PLOT1120
C     RESTORES FORMAT                                                    PLOT1130
   39 DO 40 IL=1,18                                                      PLOT1140
   40 A(IL)=C                                                            PLOT1150
   41 CONTINUE                                                           PLOT1160
C     DRAWS BOTTOM AXIS                                                  PLOT1170
      DO 42 I=1,18                                                       PLOT1180
   42 A(I)=0                                                             PLOT1190
```

```
      WRITE (NOUT,43)(A(I),I=1,18)                                    PLOT1200
   43 FORMAT(12X,18A6)                                                PLOT1210
C     RESTORES A ARRAY TO BLANKS                                      PLOT1220
      DO 44 I=1,18                                                    PLOT1230
   44 A(I)=C                                                          PLOT1240
C     SETS UP * EVERY 10 PLACES FOR LOWER AXIS                        PLOT1250
      DO 45 I=2,12,5                                                  PLOT1260
      NA(I)=NA(I)+NB(4)                                               PLOT1270
      NA(I+2)=NA(I+2)+NB(2)                                           PLOT1280
   45 NA(I+3)=NA(I+3)+NB(6)                                           PLOT1290
      NA(17)=NA(17)+NB(4)                                             PLOT1300
      NA(1)=NA(1)+NB(1)                                               PLOT1310
      WRITE (NOUT,43)(A(I),I=1,18)                                    PLOT1320
      DELTAX=((XMAX-XMIN)/FLOAT(N1))*10.0                             PLOT1330
      DO 46 I=1,11                                                    PLOT1340
   46 A(I)=XMIN+FLOAT(I-1)*DELTAX                                     PLOT1350
      WRITE (NOUT,47)(A(I),I=2,11)                                    PLOT1360
   47 FORMAT(16X,1P10E10.4)                                           PLOT1370
      RETURN                                                          PLOT1380
      END                                                             PLOT1390
END OF LISTING.     2 *DIAGNOSTIC* MESSAGE(S).
```

SUMMATION LH21 AND LH22 TWO CYCLES RWSULTS NO$_{T}$ nI,, BY CURRENT

REQUESTED DATA FROM LIBRARY TAPE

RUN LH21 CYCLE 1 REF. POINT 1

RUN LH21 CYCLE 2 REF. POINT 1

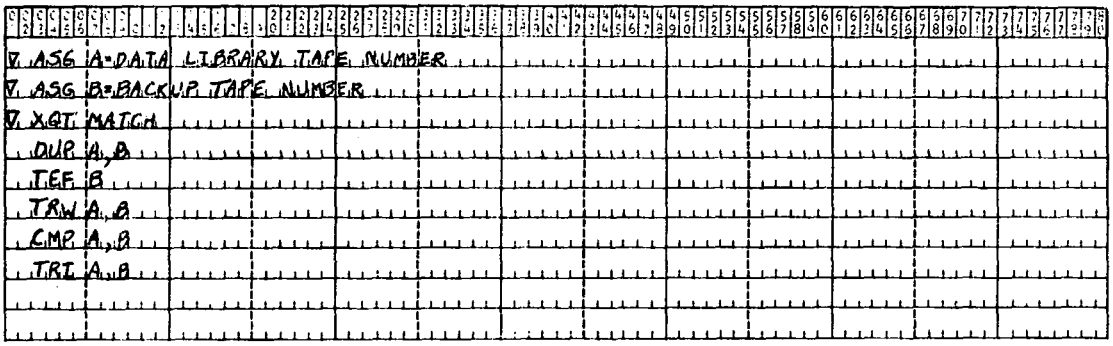
RUN LH22 CYCLE 1 REF. POINT 1

RUN LH22 CYCLE 3 REF. POINT 1

## STEP 5: COPY

The COPY program is used to make a backup tape for the data library tape. A backup tape is kept at all times. It is suggested that after every ten experiments, the library tape be copied onto the backup tape.

Below is a complete set of cards that comprise the COPY deck.




After the backup tape is written, a comparison is made. If the two tapes do not match, the output listing from COPY will so indicate.

No listing is given for this program.

STEP 6: UPDATE

Using the UPDATE program, five types of changes can be made to the data library tape. These fives changes are described below.

| Type Number | Description of Change |
|---|---|
| 1 | Allows the user to change any word of the data that was on the card for TEDIT |
| 2 | Allows the user to delete an entire experiment from the library tape |
| 3 | Causes an entire cycle to be deleted from an experiment and remaining cycles to be re-sequenced |
| 4 | Allows the signal + noise, noise, and current values for a particular channel number of a cycle to be changed |
| 5 | Allows any channel number, along with its signal + noise, noise, and current values, to be deleted from any cycle of an experiment |

Card formats for the preceding changes are as follows:

Type 1

First Card

| Column | |
|---|---|
| 6 | Punch one (1) |
| 7-12 | Experiment number |

Second Card — Identical to that used for TEDIT except for information to be changed

Type 2

| Column | |
|---|---|
| 6 | Punch two (2) |
| 7-12 | Experiment number |

Type 3

| Column | |
|---|---|
| 6 | Punch three (3) |
| 7-12 | Experiment number |
| 13-18 | Cycle number |

Type 4

| Column | |
|---|---|
| 6 | Punch four (4) |
| 7-12 | Experiment number |
| 13-18 | Cycle number |
| 19-24 | Channel number |
| 25-30 | Signal + noise value |
| 31-36 | Noise value |
| 37-42 | Current value |

The last three items are always changed together; therefore, if no change is desired, the existing value must be entered.

Type 5

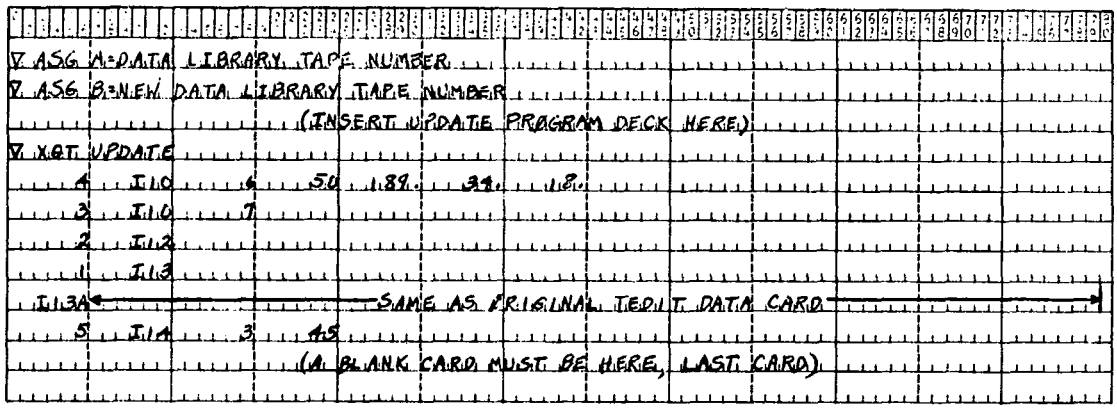
| Column | |
|---|---|
| 6 | Punch five (5) |
| 7-12 | Experimental number |
| 13-18 | Cycle number |
| 19-24 | Channel number |

The different types of change cards for any one experiment should be in the following sequence: 2, 3, and 4 (in any sequence), 5, and 1. If more than one type 5 change is to be made for any one cycle in any one experiment, cards should be in descending channel-number order, the largest first. This order eliminates the necessity of later change cards that reflect the changes made by previous change cards.

If more than one experiment is to be changed, then the individual groups of change cards must be in the same order as on the library tape (excluding experiments that are not to be changed).

Below is an example deck setup, where the data library tape consists of five experiments (I10, I11, I12, I13, and I14) and the following changes are to be made:

1. Change the signal + noise value of channel number 50 in cycle 6 of experiment I10. The values of noise and current were originally 34 and 18, respectively.
2. Delete cycle 7 of experiment I10.
3. Delete experiment I12.
4. Change run number from I13 to I13A.
5. Delete channel number 45 in cycle 3 of experiment I14.




A program listing follows.

```
@ FOR UDATE,UPDATE
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 21 JUN 68 AT 17:09:44

   MAIN PROGRAM          ENTRY POINT 000000

 1.          PARAMETER LTAPE = 9, NTAPE = 10
 2.          INTEGER CHAN, CYCLE
 3.          REAL NOISE
 4.          COMMON IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST, TINT, SIGMIN,
 5.         *   SIGMAX, CURMIN, CURMAX, DATE(2), CHAN(100,100), SPLUSN(100,,00)
 6.         * , NOISE(100,100), CURR(100,100), CYCLE(100), L(100), LAST(100)
 7.         * , NMAX
 8.          REWIND LTAPE
 9.          REWIND NTAPE
10.          CALL INRUN(LTAPE)
11.    C.. READ A CHANGE TYPE CARD..
12.       10 READ(5,11) ITYPE, NRUN, NCYC, NCHAN, XSPN, XN, XCURR
13.       11 FORMAT( I6, A6, I6, I6, 3F6.0 )
14.          IF(ITYPE.EQ.0) GO TO 80
15.       20 IF(NRUN.EQ.IRUN) GO TO 25
16.    C.. WRITE OUT RUN THAT IS IN MEMORY..
17.          CALL OUTRUN(NTAPE)
18.    C.. WAS THIS THE LAST RUN ON LTAPE?
19.          IF(LAST(NMAX).EQ.2) GO TO 110
20.    C.. READ IN A NEW RUN..
21.          CALL INRUN (LTAPE)
```

```
      GO TO 20
C.. DETERMINE WHICH TYPE OF CHANGE IS TO BE MADE..
   25 GO TO (30, 40, 50, 60, 70), ITYPE
C..   MAIN DATA IS TO BE CHANGED. TYPE 1.
   30 READ(5,31) IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST, TINT, SIGMIN,
     *  SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
   31 FORMAT( 2A6, F6.0, A6, 8F6.0, A6, A1 )
      GO TO 10
C
C.. DELETE THE RUN NOW IN MEMORY.. TYPE 2.
   40 IF(LAST(NMAX).EQ.2) GO TO 100
C.. READ IN ANOTHER RUN FROM TAPE.
      CALL INRUN(LTAPE)
      GO TO 10
C.. DELETE CYCLE NCYC WHICH IS NOW IN MEMORY. TYPE 3.
C.. CYCLE NUMBERS WILL BE RE-SEQUENCED IN OUTRUN.
   50 IF(NCYC.LE.0.OR.NCYC.GT.NMAX) GO TO 130
      CYCLE(NCYC) = 0
      GO TO 10
C.. CHANGE DATA OF CYCLE NUMBER NCYC AND CHANNEL NUMBER NCHAN.  TYPE 4.
   60 IF(NCYC.LE.0.OR.NCYC.GT.NMAX) GO TO 130
      KCHAN=NCHAN+1
      CHAN(KCHAN,NCYC) = NCHAN
      SPLUSN(KCHAN,NCYC) = XSPN
      NOISE(KCHAN,NCYC)  = XN
```

```
      CURR(KCHAN,NCYC) =  XCURR
      GO TO 10
C.. CHANNEL NUMBER NCHAN IN CYCLE NCYC IS TO BE DELETED. TYPE 5.
   70 IF(NCYC.LE.0.OR.NCYC.GT.NMAX) GO TO 130
      IF(NCHAN+1.EQ.L(NCYC))GO TO 78
      JM = L(NCYC)
      JP1 = NCHAN + 2
      DO 75 I=JP1,JM
C..   CHAN(I-1,NCYC) = CHAN(I,NCYC)
      SPLUSN(I-1,NCYC) = SPLUSN(I,NCYC)
      NOISE(I-1,NCYC) = NOISE(I,NCYC)
   75 CURR(I-1,NCYC) = CURR(I,NCYC)
   78 L(NCYC) = L(NCYC) - 1
      GO TO 10
C.. WRITE OUT THE RUN THAT IS IN MEMORY.
   80 CALL OUTRUN (NTAPE)
C.. THERE ARE NO MORE CHANGES TO BE MADE, COPY REST OF LTAPE.
   90 IF(LAST(NMAX).EQ.2) GO TO 100
      CALL INRUN(LTAPE)
      CALL OUTRUN(NTAPE)
      GO TO 90
  100 BACKSPACE NTAPE
      LAST(NMAX) = 2
      WRITE(NTAPE) LAST(NMAX)
      END FILE NTAPE
```

```
      CALL REWI(LTAPE)
      REWIND NTAPE
      CALL EXIT
  110 WRITE(6,111) NRUN
  111 FORMAT( /, 33H REQUESTED CHANGE FOR RUN NUMBER , A6, 57H IS NOT IN
     * SEQUENCE OR THE RUN NUMBER ITSELF IS IN ERROR. /  )
      GO TO 100
  130 WRITE(6,131) NCYC, NRUN
  131 FORMAT( /, 14H CYCLE NUMBER , I6,25H IS OUT OF RANGE FOR RUN A6 /)
      GO TO 100
      END
```

END OF LISTING.  0 *DIAGNOSTIC* MESSAGE(S).

```
@ FOR INRUN,INRUN
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 21 JUN 68 AT 17:09:46

   SUBROUTINE INRUN     ENTRY POINT 000204

 1.          SUBROUTINE INRUN (LTAPE)
 2.          INTEGER CHAN, CYCLE
 3.          REAL NOISE
 4.          COMMON IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST, TINT, SIGMIN,
 5.         *   SIGMAX, CURMIN, CURMAX, DATE(2), CHAN(100,100), SPLUSN(100,100)
 6.         * , NOISE(100,100), CURR(100,100), CYCLE(100), L(100), LAST(100)
 7.         * , NMAX
 8.          READ(LTAPE) IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST,TINT, SIGMIN,
 9.         *    SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
10.          N = 0
11.    C
12.       10 N = N + 1
13.          IF(N.GT.100) GO TO 20
14.          READ(LTAPE) CYCLE(N), L(N)
15.          IMAX = L(N)
16.          READ(LTAPE) ( CHAN(I,N), SPLUSN(I,N), NOISE(I,N), CURR(I,N),I=1,
17.         *  IMAX )
18.          READ(LTAPE) LAST(N)
19.          IF(LAST(N).EQ.0) GO TO 10
20.          NMAX = N
21.          RETURN
```

```
      C  DELETE THE REMAINDER OF THIS EXPERIMENT, IT EXCEEDS 100 CYCLES.
        20 READ(LTAPE) DUMMY, IDUM
           READ(LTAPE) (DUMMY, DUMMY, DUMMY, DUMMY, I=1,IDUM)
           READ(LTAPE) ILAST
           IF(ILAST.EQ.0) GO TO 20
           NMAX = 100
           LAST(NMAX) = ILAST
        30 WRITE(6,31) IRUN
        31 FORMAT( /, 5X, A6,86H EXCEEDED 100 CYCLES, THE REMAINING CYCLES HA
          *VE BEEN DELETED *** SORRY ABOUT THAT ***,     )
           RETURN
           END
END OF LISTING,      0 *DIAGNOSTIC* MESSAGE(S),
```

```
@ FOR OUTRUN,OUTRUN
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 21 JUN 68 AT 17:09:48

   SUBROUTINE OUTRUN    ENTRY POINT 000142

 1.          SUBROUTINE OUTRUN(NTAPE)
 2.          INTEGER CHAN, CYCLE
 3.          REAL NOISE
 4.          COMMON IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST, TINT, SIGMIN,
 5.         *   SIGMAX, CURMIN, CURMAX, DATE(2), CHAN(100,100), SPLUSN(100,100)
 6.         * , NOISE(100,100), CURR(100,100), CYCLE(100), L(100), LAST(100)
 7.         * , NMAX
 8.          WRITE(NTAPE) IRUN, GAS, VAR, TIME, RES, DVOLT, VOLTST, TINT,
 9.         *  SIGMIN, SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
10.          ICYC = 0
11.       10 DO 20 N=1,NMAX
12.          IF(CYCLE(N).EQ.0) GO TO 20
13.          ICYC = ICYC + 1
14.          WRITE(NTAPE) ICYC, L(N)
15.          IMAX = L(N)
16.          WRITE(NTAPE) (CHAN(I,N), SPLUSN(I,N), NOISE(I,N), CURR(I,N), I=1,
17.         *  IMAX )
18.          WRITE(NTAPE) LAST(N)
19.       20 CONTINUE
20.          BACKSPACE NTAPE
21.          WRITE(NTAPE) LAST(NMAX)
22.          RETURN
23.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

STEP 7: LEØF (List and End of File)

One input card, in FORTRAN format (A6, I6), is necessary for execution of this program.

| Column | |
|---|---|
| 1-6 | INUM = last valid experiment number |
| 7-12 | LCYCLE = last valid cycle number |

After LEØF has encountered the last valid cycle number on the library tape, an end of file is written.

A program listing follows.

```
@ FOR LEOF,LEOP
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 07 MAY 68 AT 11:58:51

   MAIN PROGRAM          ENTRY POINT 000000

 1.    C.. THE PURPOSE OF THIS ROUTINE IS TO READ THE LIBRARY TAPE AND LIST ALL
 2.    C   DATA BY RUN NUMBER AND BY CYCLE NUMBER.
 3.          PARAMETER LTAPE = 10
 4.          INTEGER CHAN
 5.          REAL NOISE
 6.          DIMENSION CHAN(100), SPLUSN(100), NOISE(100), CURR(100), DATE(2)
 7.          REWIND LTAPE
 8.          READ(5,7) INUM, LCYCLE
 9.        7 FORMAT( A6, I6)
10.        8 READ(LTAPE) NUM, ITYPE, VAR, TIME, RES, DVOLT, VOLTST, TINT,
11.         1 SIGMIN, SIGMAX, CURMIN, CURMAX, DATE(1), DATE(2)
12.          WRITE(6,11) NUM
13.       11 FORMAT( 10X, 10HRUN NUMBER, 1X, A6, /  )
14.          WRITE(6,12) ITYPE
15.       12 FORMAT( 10X, 3HGAS, 1X, A6, / )
16.          WRITE(6,13) VAR
17.       13 FORMAT( 10X, 10HVARIANCE %, 1X, F6.2, / )
18.          WRITE(6,14) TIME
19.       14 FORMAT( 10X, 4HTIME, 1X, A6, / )
20.          WRITE(6,15) RES
21.       15 FORMAT( 10X, 4HRES, 1X, F6.2, / )
```

```
      WRITE(6,16) DVOLT
   16 FORMAT( 10X, 17HVOLTAGE INCREMENT, 1X, F6.2, / )
      WRITE(6,17) VOLTST
   17 FORMAT( 10X, 17HSTARTING VOLTAGE , 1X, F6.2, / )
      WRITE(6,18) TINT
   18 FORMAT( 10X, 14HTIME INTERVAL , F6.2, / )
      WRITE(6,19) SIGMIN
   19 FORMAT( 10X, 12HMIN. SIGNAL , F10.2, / )
      WRITE(6,20) SIGMAX
   20 FORMAT( 10X, 12HMAX. SIGNAL , F10.2, / )
      WRITE(6,21) CURMIN
   21 FORMAT( 10X, 13HMIN. CURRENT , F10.2, / )
      WRITE(6,22) CURMAX
   22 FORMAT( 10X, 13HMAX. CURRENT , F10.2, / )
      WRITE(6,23) DATE(1), DATE(2)
   23 FORMAT( 10X,  4HDATE, 1X, 2A6, / )
   10 READ(LTAPE) KOUNT, L
C
      WRITE(6,24) KOUNT
   24 FORMAT( 10X, 12HCYCLE NUMBER, 1X, I3, / )
      WRITE(6,25) L
   25 FORMAT( 10X, 16HNUMBER OF POINTS, I5, //  )
C
      READ(LTAPE) (CHAN(I), SPLUSN(I), NOISE(I), CURR(I), I=1,L )
      IF(NUM.EQ.INUM.AND.KOUNT.EQ.LCYCLE) GO TO 40
```

```
      READ(LTAPE) LAST
      IF(LAST.EQ.0) GO TO 10
      WRITE(6,31)
   31 FORMAT( 1H1 )
      IF(LAST.EQ.1) GO TO 8
      WRITE(6,28)
   28 FORMAT(/ 12H END OF FILE )
      CALL REWI(LTAPE)
      CALL EXIT
   40 LAST = 2
      WRITE(LTAPE) LAST
      END FILE LTAPE
      WRITE(6,28)
      CALL REWI(LTAPE)
      CALL EXIT
      END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

## STEP 8: SMØØTH

This program Fourier-smooths data, unfolds a given Gaussian electron energy distribution from the data, and gives the results for the derivative of the function in tabular form. The program is prepared to accept card input. The deck of cards needed is generated as one of the options in ABEAM4.

The normal output of this program, which in its present form was prepared for the study of autoionization in molecular gases, is:

1. Input data Fourier-smoothed
2. Derivative of Fourier-smoothed square root of the data
3. Derivative of Fourier-smoothed data
4. Derivative of Fourier-smoothed data with energy distribution unfolded for case 1
5. Derivative of Fourier-smoothed data with energy distribution unfolded for case 2
6. Derivative of Fourier-smoothed data with energy distribution unfolded for case 3

At present there is one graphic output, which gives the input data Fourier-smoothed once.

The input sequence and card formats are given below.

Title Card: FORTRAN format is (12A6)

| Column | |
|---|---|
| 1-72 | Title (printed at top of first page) |

First Data Card: FORTRAN format is (3I6, 3F6.0, I6)

| Column | |
|---|---|
| 6 | IN = 0: accept Y values as input<br>= 1: after reading in Y values below, read YT values and compute Y = Y - YT |
| 12 | ISTOP = 0: last problem<br>= 1: read in another title card for a new problem |
| 18 | NDEL = number of delta (Δ) values to follow |
| 19-24 | DEL (1) = Δ value(s) for unfolding |

| Column | |
|---|---|
| 25-30 | DEL (2) |
| 31-36 | DEL (3) |
| 37-42 | NMAX = 0: let program choose number of Fourier coefficients to use |
| | > 0: program is to use this number of Fourier coefficients |

Second Data Card: FORTRAN format is (3F12-4)

| Column | |
|---|---|
| 1-12 | SI = initial voltage |
| 13-24 | SF = final voltage |
| 25-36 | DX = voltage increment |

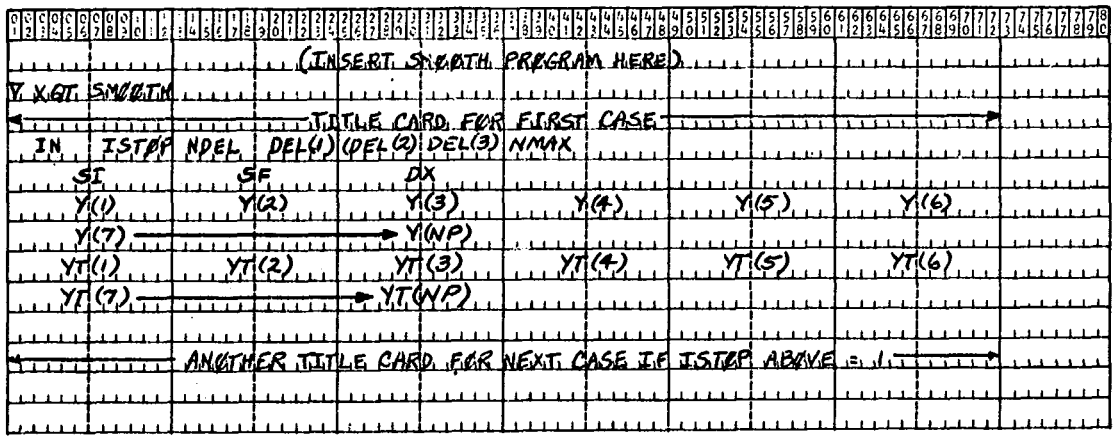
Last Data Card: FORTRAN format is (6F12. 4)

6 values per card: Y(i), i = 1, NP  NP = total number of values = [(SF - SI)/DX] + 1

YT(i), i = 1, NP  omit if IN = 0 on first data card

If this deck has been punched from the ABEAM4 program, the user must finish punching the second card (first data card) (i. e., NDEL, DEL (1), DEL (2), DEL (3), NMAX).

Below is an example deck setup.



```
@ FOR SMOOTH,SMOOTH
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 29 APR 68 AT 13:17:09

   MAIN PROGRAM          ENTRY POINT 000000
 1.   C      PROGRAM SMOOTH3
 2.          DIMENSION Y(300),YT(300),B(300),YD(300),DYS(300,3),DEL(3),YDS(300)
 3.          DIMENSION LABEL(12)
 4.          DIMENSION VOLT(100)
 5.       12 WRITE(6,124)
 6.      124 FORMAT(1H1)
 7.          READ(5,15) (LABEL(I), I=1,12)
 8.       15 FORMAT(12A6)
 9.          READ(5,16) IN, ISTOP, NDEL, DEL(1), DEL(2), DEL(3), NMAX
10.       16 FORMAT( 3I6, 3F6.0, I6 )
11.          WRITE(6,151) (LABEL(I),I=1,12)
12.      151 FORMAT(4X, 12A6 )
13.          READ (5,17)SI,SF,DX
14.       17 FORMAT(3F12.4)
15.          HL = (SF-SI)
16.          NPM = HL/DX+.1
17.          NP = NPM+1
18.          READ(5,18) (Y(I),I=1,NP)
19.       18 FORMAT(6F12.4)
20.          IF(IN)20,20,19
21.       19 READ (5,18) (YT(I),I=1,NP)
22.          DO 14 I = 1,NP
23.       14 Y(I) = Y(I)-YT(I)
24.       20 WRITE(6,174)NP,SI,DX,SF
25.      174 FORMAT(/20X,27HFOURIER SMOOTHING OF SIGNAL / 20X,30HINPUT SIGNAL F
```

```
      10K DATA RANGE... 14,1X,1H(F5.2,1H/F4.2,1H/F5.2,5H)E.V.  )
       WRITE(6,181)(Y(I),I=1,NP)
  181 FORMAT(10X,10F8.0)
       YMIN = 1.E+37
       DO 205 I=1,NP
       YMIN = AMIN1(YMIN, Y(I) )
  205 CONTINUE
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
       IF(YMIN.GE.0) GO TO 210
       DO 206 I=1,NP
       Y(I) = Y(I) - YMIN
  206 CONTINUE
  210 WRITE(6,182)
  182 FORMAT(/20X,42HFOURIER COEFFICIENTS OF SQUARE ROOT SIGNAL  /)
       X = 0.0
       YI = SQRT(Y(1))
       YF = (SQRT(Y(NP))-YI)/HL
       DO 21 I = 1,NP
       Y(I) = SQRT(Y(I))-YI-YF*X
   21 X = X+DX
       CALL FOUR(NP,Y,B)
       WRITE(6,183) (3(K),K=1,NPM)
  183 FORMAT(10X,10E10.3)
       PI = 3.141592653
       CNPM = NPM
       DO 186 I = 1,NPM
       CI = I
```

```
      186 B(I) = B(I)*COS(PI*CI/(2.0*CNPW))**2
          WRITE(6,185)
      185 FORMAT(/20X,47HFOURIER COMPONENTS FILTERED BY COS**2 ATTUATION  )
          WRITE(6,183)(B(K),K=1,NPM)
          IF(NMAX.NE.0) GO TO 35
          BT = 0.0
          DO 24 I = 1,20
          NPI = NP-I
       24 BT = BT+B(NPI)**2
          K = 20
      261 N = NP-K
          BE = B(N-1)**2
          CK = K
          BET = BT/CK
          IF(BE/BET-16.)27,27,28
       27 IF(N-2)29,29,33
       29 NMAX = NP/10
          WRITE(6,291)
      291 FORMAT(/20X,11HTEST FAILED /)
          GO TO 35
       33 K = K+1
          BT = BT+BE
          GO TO 261
       28 IF(N-25)231,33,33
      261 NMAX = N+2
       35 CONTINUE
          WRITE(6,36)NMAX
```

```
      CALL FOUR1(NMAX,NP,B,Y,YD)
   36 FORMAT(/20X,24HSMOOTHED SQUARE ROOT HAS I4,1X,18HFOURIER COMPONENT
     1S  / )
      X=0.0
      DO 37 K = 1,NP
      YK = Y(K)+YI+YF*X
      Y(K) = YK*YK
   37 X = X+DX
*DIAGNOSTIC*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
      IF(YMIN.GE.0) GO TO 44
      DO 43 I=1,NP
      Y(I) = Y(I) + YMIN
   43 CONTINUE
   44 NPMT = NP - 2
      DO 45 I =1,2
   45 YDS(I) = 0.0
      DO 46 I = 3,NPMT
   46 YDS(I) = 0.10*(-2.0*Y(I-2)-Y(I-1)+Y(I+1)+2.0*Y(I+2))
      DO465 I = NPM,NP
  465 YDS(I) = 0.0
      DO 60 J=1,NDEL
      CALL UNFSQR(NMAX,NP,HL,DEL(J),DX,YI,YF,B,YT)
      DO 40 I = 1,2
   40 DYS(I,J) = 0.0
      DO 41 I = 3,NPMT
   41 DYS(I,J) = 0.10*(-2.0*YT(I-2)-YT(I-1)+YT(I+1)+2.0*YT(I+2))
      DO 42 I = NPM,NP
```

```
      42 DYS(I,J) = 0.0
      60 CONTINUE
         WRITE(6,51)
      51 FORMAT( / 20X 26HS = INPUT DATA (SMOOTHED).  )
         WRITE(6,52)
      52 FORMAT( / 20X 57HDSA = DERIVATIVE OF (SMOOTHED SQUARE ROOT OF INPU
        *T DATA).  )
         WRITE(6,53)
      53 FORMAT( / 20X 26HDT(0) = DERIVATIVE OF (S).  )
         WRITE(6,54)
      54 FORMAT( / 20X 37HDT(.XX) = DERIVATIVE OF (UNFOLDED S).  )
         WRITE(6,61) (DEL(I), I=1,NDEL)
      61 FORMAT(    / 18X, 1HX 13X 1HS 11X 3HDSA 9X 6H DT(0) 3(7X 3HDT(,
     1  F4.2, 1H)  )  )
         X=SI
         DO 70 I = 1,NP
         WRITE(6,63) X, Y(I), YD(I), YDS(I), (DYS(I,J),J=1,NDEL)
      63 FORMAT( 10X, F9.2, 6F14.4 )
         VOLT(I) = X
      70 X = X+DX
         WRITE(6,901)
     901 FORMAT( 1H1,  33HPLOT OF S SMOOTHED ONCE (FOURIER)          )
         CALL PLOT( VOLT, Y, NP, 100, 46, 6 )
         IF(ISTOP) 72, 72, 72
      72 CALL EXIT 72, 72, 72
         END
END OF LISTING,     2 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR UNFSQR,UNFSQR
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 29 APR 68 AT 13:17:12

   SUBROUTINE UNFSQR     ENTRY POINT 000440

 1.          SUBROUTINE UNFSQR(NC,NP,HL,DL,DX,SI,SF,B,Y)
 2.          DIMENSION Y(300), B(300),C(300),S(300),EX(300)
 3.          PI = 3.141592653
 4.          TLN = 0.69314718
 5.          CHI = (PI*DL/HL)**2/(16.*TLN)
 6.          CON = SI*SI-(SF*DL)**2/(8.0*TLN)
 7.          CLOP = 2.0*CHI*HL/PI
 8.          SGN = -1.0
 9.          SU1 = 0.0
10.          SU2 = 0.0
11.          DO 60 K = 1,NC
12.          CK = K
13.          SU1 = SU1 + CK*B(K)
14.          SU2 = SU2 + SGN*CK*B(K)
15.       60 SGN = -SGN
16.          SU1 = -2.0*SF*CLOP*SU1
17.          SU2 = -2.0*SF*CLOP*SU2
18.          Y(1) = CON+SU1
19.          Y(NP)=(SF*HL)**2 +2.0*SI*SF*HL+CON+SU2
20.          NPM = NP-1
21.          X = DX
22.          SINX = SIN(PI*X/HL)
```

```
      COSX = COS(PI*X/HL)
      EC = EXP(CHI)
      FC = EC*EC
      SINZ = SINX
      COSZ = COSX
      NCM = NC-1
      NT = NC+NC
      EXPZ = 1.0
      DO 10 K =1,NT
      EXPZ = EC*EXPZ
      EX(K) = EXPZ
   10 EC = FC*EC
      DO 50 M = 2,NPM
      YM = (SF*X)**2+2.0*SF*SI*X+CON
      SINK = SINX
      COSK = COSX
      DO 20 K = 1,NT
      S(K) = SINK
      C(K) = COSK
      SINKP = SINK*COSX+COSK*SINX
      COSKP = COSK*COSX-SINK*SINX
      SINK = SINKP
   20 COSK = COSKP
      TG = 0.0
      DO 30 K = 1,NCM
```

```
      BK = 0.0
      KP = K+1
      DO 28 N = KP,NC
      NMK = N-K
      NPK = N+K
   28 BK = BK+B(N)*(EX(NMK)*C(NMK)-EX(NPK)*C(NPK))
   30 TG = TG + B(K)*BK
      TH = 0.0
      TE = 0.0
      DO 40 K = 1,NC
      CK = K
      BK = B(K)
      KT = K+K
      TG = TG+BK*BK*(1.-EX(KT)*C(KT))/2.0
      TH = TH +BK*EX(K)*(X*S(K)-CLOP*CK*C(K))
   40 TE = TE + BK*EX(K)*S(K)
      Y(M) = TG+2.0*SF*TH+2.0*SI*TE+YM
      X = X+DX
      SINK = SINX*COSZ+COSX*SINZ
      COSK = COSX*COSZ-SINX*SINZ
      SINX = SINK
   50 COSX = COSK
      RETURN
      END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOUR,FOUR
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 29 APR 68 AT 13:17:14

   SUBROUTINE FOUR      ENTRY POINT 000127

 1.          SUBROUTINE FOUR(NP,Y,B)
 2.          DIMENSION Y(300),B(300)
 3.          PI = 3.141592653
 4.          CNP = NP
 5.          NPM = NP-1
 6.          CNPM = NPM
 7.          PION = PI/CNPM
 8.          COSZ = COS(PION)
 9.          SINZ = SIN(PION)
10.          COSK = COSZ
11.          SINK = SINZ
12.          DO 20 K =1,NPM
13.          BK = 0.0
14.          COSKI = COSK
15.          SINKI = SINK
16.          DO 22 I = 2,NPM
17.          BK = BK + Y(I)*SINKI
18.          SINI = SINKI*COSK+COSKI*SINK
19.          COSI = COSKI*COSK-SINKI*SINK
20.          SINKI = SINI
21.       22 COSKI = COSI
```

```
      SINKI = SINK*COSZ+COSK*SINZ
      COSKI = COSK*COSZ-SINK*SINZ
      COSK =COSKI
      SINK =SINKI
   20 B(K)=2.0*BK/CNP
      RETURN
      END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOURI,FOURI
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 29 APR 68 AT 13:17:15

   SUBROUTINE FOURI      ENTRY POINT 000145

 1.          SUBROUTINE FOURI(NMAX,NP,B,Y,YD)
 2.          DIMENSION B(300),Y(300),YD(300)
 3.          NPM = NP-1
 4.          CNPM = NPM
 5.          PI = 3.141592653
 6.          PIOM = PI/CNPM
 7.          COSZ = COS(PIOM)
 8.          SINZ = SIN(PIOM)
 9.          Y(1) = 0.0
10.          YD(1) = 0.0
11.          COSK = COSZ
12.          SINK = SINZ
13.          DO 20 K = 2,NP
14.          YK = 0.0
15.          YDK = 0.0
16.          PIK = PIOM
17.          COSKI = COSK
18.          SINKI = SINK
19.          DO 22 I =1,NMAX
20.          YK = YK+B(I)*SINKI
21.          YDK = YDK + PIK*B(I)*COSKI
```

```
      PIK = PIK+PIOM
      SINI = SINKI*COSK+COSKI*SINK
      COSI = COSKI*COSK-SINKI*SINK
      COSKI = COSI
      SINKI = SINI
   22 CONTINUE
      COSKI = COSK*COSZ-SINK*SINZ
      SINKI = COSK*SINZ+SINK*COSZ
      COSK = COSKI
      SINK = SINKI
      Y(K) = YK
   20 YO(K)= YDK
      RETURN
      END
```

END OF LISTING. 0 *DIAGNOSTIC* MESSAGE(S).

STEP 9: SIMCUR

The program is designed to fold into any given analytic function a Gaussian function with specified full width at half maximum, $\Delta$, in eV units:

$$F(E) = \frac{1}{N} \int_{x_0}^{x_L} f(E') \exp\left[-\ell n \frac{2}{(1/2\,\Delta)^2} (E - E')^2\right] dE'$$

where the normalization function is

$$N = \int_{x_0}^{x_L} \exp\left[-\ell n \frac{2}{(1/2\,\Delta)^2} (E - E')^2\right] dE' \quad .$$

In program notation the function is

$$CS(i) = \frac{\int_{x_0}^{x_L} CS(x) * \exp[-\xi(E - x)^2]\, dx}{\int_{x_0}^{x_L} \exp[-\xi(E - x)^2]\, dx} \quad ,$$

where

$$\xi = \frac{LN(2)}{\left(\frac{1}{2}\,\Delta/13.605\right)^2}$$

$$E = \frac{EV(i)}{13.605}$$

$$X_0 = E - LIMITS$$

$$X_L = E + LIMITS$$

$$EV(i) = EVMIN + (i - 1) * DELEV \quad .$$

The output of this program is in table form giving the energy scale in eV and Rydberg units. As an option the output can be given in graphic form.

In the case considered here, the form of the ionization cross section proposed by Omidvar is in the program. This equation can be replaced by any other. In its present form it is possible to obtain as an option the ratio of Omidvar's function to any requested power function. The input card formats are as follows:

First Card: FORTRAN format is (2E12.6, 3I6)

| Column | |
|---|---|
| 1-12 | COE = coefficient of power function |
| 13-24 | POWER = power of the function |
| 25-36 | KLAST = 1: return for new run |
| | = 2: exit; all job completed |

Second Card: FORTRAN format is (2E12.6, 3I6)

| Column | |
|---|---|
| 1-12 | LIMITS = integration interval |
| 13-24 | DELTA = full width at half maximum of Gaussian distribution |
| 25-30 | IFOLD = 1: do not fold data |
| | = 2: fold data |
| 31-36 | IPLOT = 1: give plot |
| | = 2: do not give plot |
| 37-42 | ILAST = 1: return here for new set of options after processing this problem |
| | = 2: do not return here |

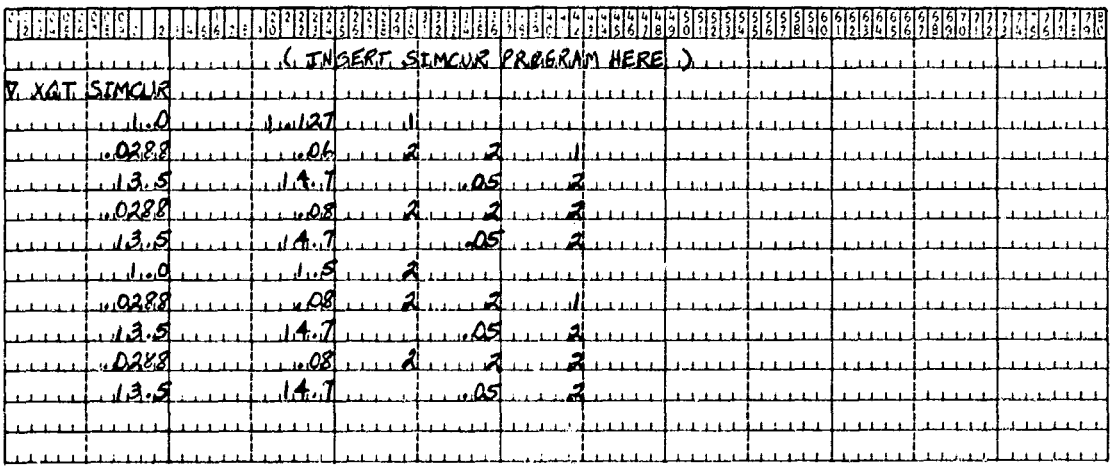
Third Card: FORTRAN format is (3E12.6, I6)

| Column | |
|---|---|
| 1-12 | EVMIN = the minimum value of the electron energy (eV) in the domain of the problem |
| 13-24 | EVMAX = the maximum value of the electron energy (eV) in the problem |
| 25-36 | DELEV = the step for output starting at EVMIN and going to EVMAX |

37-42 LAST = 1: return here for new values after processing this problem

= 2: do not return here

Below is an example of the deck setup as it stands for the Omidvar equation. In this case we are comparing Omidvar's cross section first with the 1.127 power law and then with a 1.5 power law. A plot is not requested. The energy distributions requested are 0.06 eV and 0.08 eV.




A program listing follows.

```
@ FOR SIMCUR,SIMCUR
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:03

   MAIN. PROGRAM          ENTRY POINT 000000

  1.   C     PLOT SIMPLE CURVE AND FOLD SIMPLE CURVE
  2.         DIMENSION CS(1000), EV(1000), ARRAY(20)
  3.         COMMON    /SIGMA/ COE, POWER
  4.         COMMON    /FUN/ XSEE, XK
  5.         DATA INIT/ -1/, IPEND/1/
  6.         REAL LIMITS
  7.         IP = 2
  8.   C
  9.   C... COE IS NOT USED IN OMIDVAR'S FUNCTION, INPUT CARD IS TO BE
 10.   C... LEFT BLANK IN THIS FIELD.
 11.     400 READ(5,401) COE, POWER, KLAST
 12.     401 FORMAT( 2E12.6,3I6)
 13.     410 READ(5,401) LIMITS, DELTA, IFOLD, IPLOT, ILAST
 14.   C     SET LINE COUNTER
 15.         LC = 60
 16.   C
 17.         XSEE = .69315/(.5*DELTA/13.605)**2
 18.   C     READ INTEGRATION GRID DEFINITIONS.
 19.     420 READ(5,421) EVMIN, DELEV, EVMAX, LAST
 20.     421 FORMAT( 3E12.6, I6 )
 21.         I = 0
 22.         GO TO (450, 550), IFOLD
 23.   C     SIMPLE CURVE........
```

```
      450 YMAX =1.E-37
      500 I = I + 1
          IF(I.GT.1000) GO TO 900
          IF(I.GT.1) GO TO 505
          EV(1) = EVMIN
          GO TO 507
      505 EV(I) = EV(I-1) + DELEV
      507 XK = EV(I)/13.605
          CALL CROSS(XK, CS(I))
          YMAX = AMAX1(YMAX, CS(I))
          IF(LC.LT.54) GO TO 520
      510 WRITE(6,511)
      511 FORMAT( 1H1, 39X 25 H SIMPLE CURVE - OMIDVAR -  // 54X 2HEV, 19X,
     1  1HK, 18X, 2HCS )
          CALL BCDCON(ARRAY)
          WRITE(0,515)
      515 FORMAT(24HSIMPLE CURVE - OMIDVAR -  72X  )
          LC = 3
      520 WRITE(6,521) EV(I), XK, CS(I)
      521 FORMAT( 36X, 3E20.8 )
          LC = LC + 1
          IF(ABS(EV(I)-EVMAX)-.001) 700, 700, 500
C
C     FOLDED CURVE.........
      550 YMAX = 1.E-37
      600 I = I + 1
          IF(I.GT.1000) GO TO 900
```

```
      IF(I.GT.1) GO TO 605
      EV(1) = EVMIN
      GO TO 607
  605 EV(I) = EV(I-1) + DELEV
  607 XK = EV(I)/13.605
      XO = XK - LIMITS
      XL = XK + LIMITS
      NP = 1
      REL = .01
      CALL GAUSS(INIT, XO, XL, Y1, REL, NP, 1)
      NP = 1
      REL = .01
      CALL GAUSS(INIT, XO, XL, Y2, REL, NP, 2)
      CS(I) = Y1/Y2
      YMAX = AMAX1(YMAX,CS(I))
      IF(LC.LT.54) GO TO 620
  610 WRITE(6,611) DELTA, LIMITS
  611 FORMAT( 1H1, 9X, 25HFOLDED CURVE USING DELTA= , F10.5, 9H, LIMITS=
     1  F10.5, 12H - OMIDVAR - // 54X, 2HEV, 19X, 1HK, 18X, 2HCS )
      CALL BCDCON(ARRAY)
      WRITE(0,615) DELTA, LIMITS
  615 FORMAT( 25HFOLDED CURVE USING DELTA= , F10.5,  8H LIMITS= , F10.5,
     1  12H - OMIDVAR -  31X )
      LC = 3
  620 WRITE(6,521) EV(I), XK, CS(I)
      LC = LC + 1
      IF(ABS(EV(I)-EVMAX)-.001) 700, 700, 600
```

```
C
C     THIS GRID COMPLETE..
  700 GO TO(420, 710), LAST
C     THIS FOLD COMPLETE. CHECK FOR PLOT.
  710 GO TO (720, 750), IPLOT
  720 IF(IPEND.GT.1) GO TO 730
      CALL SETUP( 0.0, 0, 16)
      IPEND = 2
      IP = 1
  730 CALL ADF
      CALL DGA(123,766,0,900, 13.45, 14.45, YMAX, 0.0 )
      CALL OUTLIN
      CALL  DRG(5,7)
      CALL SBLIN(5,9)
      CALL SLLIN(7,9)
      II=I-1
      CALL DVR(II,1,EV,CS,1)
C...  LABEL GRAPH
      CALL CONX (1, XPT)
      CALL CONY (1000, YPT)
      CALL TSP (XPT, YPT, ARRAY, 96)
C     CHECK FOR NEXT IFOLD
  750 GO TO (410, 760), ILAST
C     THIS CURVE COMPLETE
  760 GO TO (400, 770), KLAST
C     END OF JOB
  770 GO TO (780, 800), IP
```

```
105.   C     CLOSE OUT PLOT ROUTINE
106.       780 CALL FINISH
107.       800 STOP
108.       900 WRITE(6,901)
109.       901 FORMAT(113H CHECK INPUT VALUE FOR EVMIN, EVMAX AND DELEV, ONE OF T
110.          1HEM IS IN ERROR AND WILL CAUSE RESERVED STORAGE OVERFLOW.    )
111.           IF(IPEND.EQ.1) STOP
112.           IP = 2
113.           GO TO 770
114.           END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR GAUSS,GAUSS
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:07

   SUBROUTINE GAUSS     ENTRY POINT 000317

 1.         SUBROUTINE GAUSS(INIT, XO, XL, Y, REL, NP, IFUN)
 2.         DIMENSION AA(16), HH(16), YBAR(10), BYB(10)
 3.         IF(INIT) 1, 1, 2
 4.       1 INIT = 1
 5.         AA(1) = -.989400935
 6.         AA(2) = -.944575023
 7.         AA(3) = -.865631202
 8.         AA(4) = -.755404408
 9.         AA(5) = -.617876244
10.         AA(6) = -.458016778
11.         AA(7) = -.281603551
12.         AA(8) = -.950125098E-01
13.         AA(9) = -AA(8)
14.         AA(10)= -AA(7)
15.         AA(11)= -AA(6)
16.         AA(12)= -AA(5)
17.         AA(13)= -AA(4)
18.         AA(14)= -AA(3)
19.         AA(15)= -AA(2)
20.         AA(16)= -AA(1)
21.         HH(1) =  .27152459E-01
```

```
      HH(2) =  .62253524E-01
      HH(3) =  .95158512E-01
      HH(4) =  .12462897
      HH(5) =  .14959599
      HH(6) =  .16915652
      HH(7) =  .18260342
      HH(8) =  .18945061
      HH(9) =  HH(8)
      HH(10)=  HH(7)
      HH(11)=  HH(6)
      HH(12)=  HH(5)
      HH(13)=  HH(4)
      HH(14)=  HH(3)
      HH(15)=  HH(2)
      HH(16)=  HH(1)
      NG    =  16
C
    2 Y = 0.0
      XLGTH = XL - X0
      IF(XLGTH) 201, 105, 201
  201 NPP = NP
      DO 103 K=1,10
      Y = 0.
      ENP = NP
      DO 200 L=1,NP
```

```
      AREA = 0.0
      AL = L
      X1PX2 =  (2.0*AL - 1.0)*XLGTH/ENP + 2.0*XO
      X2MX1 =  XLGTH/ENP
      DO 100 J=1,NG
      X = (X1PX2 + AA(J)*X2MX1)/2.0
      CALL FOFX( X, FX, IFUN)
  100 AREA = AREA + HH(J)*FX
      Y = Y + AREA
  200 CONTINUE
      Y = XLGTH/(2.0*ENP)*Y
      YBAR(K) = Y
      IF(K-1) 104, 104, 144
  144 BYB(K-1) = ABS(YBAR(K-1) - Y)
      IF(BYB(K-1) - REL*ABS(Y)) 105, 105, 104
  104 NP = 2*NP
  103 CONTINUE
      DO 108 L=1,10
      REL = 2.0*REL
      DO 107 K=2,10
      IF(BYB(K-1) - REL*ABS(YBAR(K))) 106, 106, 107
  107 CONTINUE
  108 CONTINUE
      K = 10
  106 NP = (2**(K-1))*NPP
```

```
 72.          Y = YBAR(K)
 73.      105 RETURN
 74.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOFX,FOFX
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:11

   SUBROUTINE FOFX      ENTRY POINT 000033
1.          SUBROUTINE FOFX( X, FX, IFUN)
2.    C     EVALUATE ONE OF TWO FUNCTIONS FOR GAUSS.
3.          COMMON /FUN/ XSEE, E`
4.          FX = EXP(-XSEE*(E-X)**2)
5.          GO TO (100, 200), IFUN
6.      100 CALL CROSS(X, CS)
7.          FX = FX*CS
8.      200 RETURN
9.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR CROSS,CROSS
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:13

   SUBROUTINE CROSS     ENTRY POINT 000122

 1.          SUBROUTINE CROSS (E, CS )
 2.          COMMON   /SIGMA/ COE, POWER
 3.    C.
 4.    C...  OMIDVAR
 5.    C
 6.          REAL NU
 7.          VALUE = E - 1.0
 8.          IF(VALUE) 100, 100, 200
 9.      100 CS = 0.0
10.          RETURN
11.      200 NU = 1.0/(SQRT(E)+1.0)
12.          F1 = 16.0*NU
13.          F2 = 3.0 - F1*NU
14.          F3 = 2.0*NU*ALOG(4.0*VALUE)
15.          CS = 6.0*NU*(1.0 + 3.0*(F2*COS(F3) + F1*SIN(F3))/(F2**2 + F1**2))
16.         1     *VALUE**1.5/(TANH(3.14159265*NU)*.014)
17.          IF(POWER) 210, 220, 210
18.      210 CS = CS/VALUE**POWER
19.      220 RETURN
20.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

STEP 10: SIMTAB

This program is designed to fold a Gaussian function into any given function which has been prepared in table form. This program is identical to SIMCUR except the term CS(x) is interpolated from tabular data.

It is not necessary that the input be given in equal intervals. Within the program is an interpolation subroutine that can be as much as a ninth-order polynomial.

The input card formats are as follows:

First Card: FORTRAN format is (2I6)

| Column | |
|---|---|
| 1-6 | NL = number of points in the table (max 100) |
| 7-12 | KLAST = 1: return here for new table |
| | = 2: exit; all jobs finished |

Table Cards: FORTRAN format is (6E12.6)

| Column | |
|---|---|
| 1-12 | XX(1) = first energy value |
| 13-24 | YY(1) = first cross section value |
| 25-36 | XX(2) |
| 37-48 | YY(2) |
| 49-60 | XX(3) |
| 61-72 | YY(3) |

Continue with three pairs per card.

Next Card after Table: FORTRAN format is (2E12.6, 3I6)

| Column | |
|---|---|
| 1-12 | LIMITS |
| 13-24 | DELTA |
| 25-30 | IFOLD |
| 31-36 | IPLOT |
| 37-42 | ILAST |

Next Card: FORTRAN format is (3E12.6, I6)

| Column | |
|---|---|
| 1-12 | EVMIN |
| 13-24 | DELEV |
| 25-36 | EVMAX |
| 37-42 | LAST |

The last two cards are identical to cards two and three for the SIMCUR program.

A program listing follows.

```
@ FOR SIMTAB,SIMTAB
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:16

   MAIN PROGRAM          ENTRY POINT 000000

 1.   C      PLOT SIMPLE CURVE AND FOLD SIMPLE CURVE
 2.          DIMENSION CS(1000), EV(1000), ARRAY(20)
 3.          DIMENSION XX(100), YY(100)
 4.          COMMON /SIGMA/ NL, XX, YY
 5.          COMMON     /FUN/ XSEE, XK
 6.          DATA INIT/ -1/, IPEND/1/
 7.          REAL LIMITS
 8.          IP = 2
 9.   C
10.          ITAB = 0
11.      400 READ(5,406) NL, KLAST
12.      406 FORMAT( 2I6 )
13.          READ(5,407) (XX(I), YY(I), I=1,NL )
14.      407 FORMAT(6E12.6 )
15.          ITAB = ITAB + 1
16.          DO 408 I=1,NL
17.      408 XX(I) = XX(I)/13.605
18.      401 FORMAT( 2E12.6,3I6)
19.      410 READ(5,401) LIMITS, DELTA, IFOLD, IPLOT, ILAST
20.   C      SET LINE COUNTER
21.          LC = 60
22.   C
```

```
      XSEE = .69315/(.5*DELTA/13.605)**2
C     READ INTEGRATION GRID DEFINITIONS.
  420 READ(5,421) EVMIN, DELEV, EVMAX, LAST
  421 FORMAT( 3E12.6, I6 )
      I = 0
      GO TO (450, 550), IFOLD
C     SIMPLE CURVE.....
  450 YMAX = 1.E-37
  500 I = I + 1
      IF(I.GT.1000) GO TO 900
      IF(I.GT.1) GO TO 505
      EV(1) = EVMIN
      GO TO 507
  505 EV(I) = EV(I-1) + DELEV
  507 XK = EV(I)/13.605
      CALL CROSS(XK, CS(I))
      YMAX = AMAX1(YMAX, CS(I))
      IF(LC.LT.54) GO TO 520
  510 WRITE(6,511) ITAB
  511 FORMAT( 1H1, 39X 41H SIMPLE CURVE   SIGMA = FUNCTION OF TABLE I3
     1 // 54X 2HEV 19X 1HK 18X 2HCS )
      CALL BCDCON(ARRAY)
      WRITE(0,515) ITAB
  515 FORMAT(40HSIMPLE CURVE  SIGMA = FUNCTION OF TABLE  I3, 53X )
      LC = 3
  520 WRITE(6,521) EV(I), XK, CS(I)
  521 FORMAT( 36X, 3E20.8 )
```

```
      LC = LC + 1
      IF((EV(I)+DELEV).LT.EVMAX) GO TO 500
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
      IF(EV(I).GE.EVMAX) GO TO 700
      IF((I+1).GT.1000) GO TO 900
      I = I + 1
      EV(I) = EVMAX
      GO TO 507
C
C     FOLDED CURVE........
  550 YMAX = 1.E-37
  600 I = I + 1
      IF(I.GT.1000) GO TO 900
      IF(I.GT.1) GO TO 605
      EV(1) = EVMIN
      GO TO 607
  605 EV(I) = EV(I-1) + DELEV
  607 XK = EV(I)/13.605
      XO = XK - LIMITS
      XL = XK + LIMITS
      NP = 1
      REL = .01
      CALL GAUSS(INIT, XO, XL, Y1, REL, NP, 1)
      NP = 1
      REL = .01
      CALL GAUSS(INIT, XO, XL, Y2, REL, NP, 2)
      CS(I) = Y1/Y2
```

```
      YMAX = AMAX1(YMAX,CS(I))
      IF(LC.LT.54) GO TO 620
  610 WRITE(6,611) DELTA, LIMITS, ITAB
  611 FORMAT(1H1, 9X,  25HFOLDED CURVE USING DELTA= , F10.5,  9H, LIMITS
     1=, F10.5,  27H SIGMA = FUNCTION OF TABLE  I3  //
     2 54X, 2HEV, 19X, 2HK, 18X, 2HCS )
      CALL BCDCON(ARRAY)
      WRITE(0,615) DELTA, LIMITS, ITAB
  615 FORMAT( 25HFOLDED CURVE USING DELTA= , F10.5,  8H LIMITS= , F10.5,
     1 27H SIGMA = FUNCTION OF TABLE  I3  )
      LC = 3
  620 WRITE(6,521) EV(I), XK, CS(I)
      LC = LC + 1
      IF((EV(I)+DELEV).LT.EVMAX) GO TO 600
*DIAGNOSTIC*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
      IF(EV(I).GE.EVMAX) GO TO 700
      IF((I+1).GT.1000) GO TO 900
      I = I + 1
      EV(I) = EVMAX
      GO TO 607
C
C     THIS GRID COMPLETE..
  700 GO TO(420, 710), LAST
C     THIS FOLD COMPLETE. CHECK FOR PLOT.
  710 GO TO (720, 750), IPLOT
  720 IF(IPEND.GT.1) GO TO 730
      CALL SETUP( 0.0, 0, 16)
```

```
      IPEND = 2
      IP = 1
  730 CALL ADF
      XX1 = XX(1)*13.605
      XXNL = XX(NL)*13.605
      CALL DGA( 123, 766, 0, 900, XX1, XXNL, YMAX, 0.0 )
      CALL OUTLIN
      CALL  DRG(5,7)
      CALL SBLIN(5,9)
      CALL SLLIN(7,9)
      II=I-1
      CALL DVR(II,1,EV,CS,1)
C...  LABEL GRAPH
      CALL CONX (1, XPT)
      CALL CONY (1000, YPT)
      CALL TSP (XPT, YPT, ARRAY, 96)
C     CHECK FOR NEXT IFOLD
  750 GO TO (410, 760), ILAST
C     THIS CURVE COMPLETE
  760 GO TO (400, 770), KLAST
C     END OF JOB
  770 GO TO (780, 800), IP
C     CLOSE OUT PLOT ROUTINE
  780 CALL FINISH
  800 STOP
  900 WRITE(6,901)
  901 FORMAT(113H CHECK INPUT VALUE FOR EVMIN, EVMAX AND DELEV, ONE OF T
```

```
129.          1HEM IS IN ERROR AND WILL CAUSE RESERVED STORAGE OVERFLOW.    )
130.           IF(IPEND.EQ.1) STOP
131.           IP = 2
132.           GO TO 770
133.           END
END OF LISTING.      2 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR GAUSS,GAUSS
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:20

   SUBROUTINE GAUSS     ENTRY POINT 000317

1.          SUBROUTINE GAUSS(INIT, XO, XL, Y, REL, NP, IFUN)
2.          DIMENSION AA(16), HH(16), YBAR(10), BYB(10)
3.          IF(INIT) 1, 1, 2
4.        1 INIT = 1
5.          AA(1) = -.989400935
6.          AA(2) = -.944575023
7.          AA(3) = -.865631202
8.          AA(4) = -.755404408
9.          AA(5) = -.617876244
10.         AA(6) = -.458016778
11.         AA(7) = -.281603551
12.         AA(8) = -.950125098E-01
13.         AA(9) = -AA(8)
14.         AA(10)= -AA(7)
15.         AA(11)= -AA(6)
16.         AA(12)= -AA(5)
17.         AA(13)= -AA(4)
18.         AA(14)= -AA(3)
19.         AA(15)= -AA(2)
20.         AA(16)= -AA(1)
21.         HH(1) =  .27152459E-01
22.         HH(2) =  .62253524E-01
```

```
      HH(3) =  .95158512E-01
      HH(4) =  .12462897
      HH(5) =  .14959599
      HH(6) =  .16915652
      HH(7) =  .18260342
      HH(8) =  .18945061
      HH(9) =  HH(8)
      HH(10)=  HH(7)
      HH(11)=  HH(6)
      HH(12)=  HH(5)
      HH(13)=  HH(4)
      HH(14)=  HH(3)
      HH(15)=  HH(2)
      HH(16)=  HH(1)
      NG    =  16
C
    2 Y = 0.0
      XLGTH = XL - XO
      IF(XLGTH) 201, 105, 201
  201 NPP = NP
      DO 103 K=1,10
      Y = 0.
      ENP = NP
      DO 200 L=1,NP
      AREA = 0.0
      AL = L
```

```
      X1PX2 =  (2.0*AL - 1.0)*XLGTH/ENP + 2.0*XO
      X2MX1 =  XLGTH/ENP
      DO 100 J=1,NG
      X = (X1PX2 + AA(J)*X2MX1)/2.0
      CALL FOFX( X, FX, IFUN)
  100 AREA = AREA + HH(J)*FX
      Y = Y + AREA
  200 CONTINUE
      Y = XLGTH/(2.0*ENP)*Y
      YBAR(K) = Y
      IF(K-1) 104, 104, 144
  144 BYB(K-1) = ABS(YBAR(K-1) - Y)
      IF(BYB(K-1) - REL*ABS(Y)) 105, 105, 104
  104 NP = 2*NP
  103 CONTINUE
      DO 108 L=1,10
      REL = 2.0*REL
      DO 107 K=2,10
      IF(BYB(K-1) - REL*ABS(YBAR(K))) 106, 106, 107
  107 CONTINUE
  108 CONTINUE
      K = 10
  106 NP = (2**(K-1))*NPP
      Y = YBAR(K)
  105 RETURN
      END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR FOFX,FOFX
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:23


   SUBROUTINE FOFX      ENTRY POINT 000033
1.          SUBROUTINE FOFX( X, FX, IFUN)
2.    C     EVALUATE ONE OF TWO FUNCTIONS FOR GAUSS.
3.          COMMON /FUN/ XSEE, E
4.          FX = EXP(-XSEE*(E-X)**2)
5.          GO TO (100, 200), IFUN
6.      100 CALL CROSS(X, CS)
7.          FX = FX*CS
8.      200 RETURN
9.          END
END OF LISTING.      0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR CROSS,CROSS
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G14B
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:26

   SUBROUTINE CROSS     ENTRY POINT 000034
 1.          SUBROUTINE CROSS (E,CS )
 2.          DIMENSION XX(100), YY(100)
 3.          COMMON /SIGMA/ NL, XX, YY
 4.          IF(YY(1)) 10, 10, 17
 5.       10 IF(E-XX(2)) 15, 16, 17
 6.       15 CS = 0
 7.          RETURN
 8.       16 CS = YY(2)
 9.          RETURN
10.       17 CS = TERP( XX, YY, NL, E, 3)
11.          IF(CS.LT.0.) CS = 0.0
12.          RETURN
13.          END
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

```
@ FOR TERP,TERP
UNIVAC 1108 FORTRAN IV LEVEL  2201 0029 F4G148
THIS COMPILATION WAS DONE ON 27 MAY 68 AT 11:58:29

   FUNCTION TERP        ENTRY POINT 000267

 1.         FUNCTION TERP(X,Y,NL,ARG,IL)                                  TERP0010
 2.    C----------------------------------------------------------------------TERP0020
 3.    C     THIS FUNCTION DOES LAGRANGIAN INTERPOLATION OR                 TERP0030
 4.    C     EXTRAPOLATION OF ILTH ORDER ON X AND Y FOR ARG                 TERP0040
 5.    C     WHEN THE TABLES ARE EITHER INCREASING OR DECREASING            TERP0050
 6.    C----------------------------------------------------------------------TERP0060
 7.    C     X             X ARRAY, INDEPENDENT VARIABLE                    TERP0070
 8.    C     Y             Y ARRAY, DEPENDENT VARIABLE                      TERP0080
 9.    C     NL            NUMBER OF ENTRIES IN TABLES OF X AND Y           TERP0090
10.    C     ARG           INDEPENDENT VARIABLE VALUE                       TERP0100
11.    C     IL            NUMBER OF POINTS TO USE FOR INTERPOLATION        TERP0110
12.    C----------------------------------------------------------------------TERP0120
13.         DIMENSION X(2),Y(2)                                            TERP0130
14.    C    DIMENSION X(2),Y(2)                                            TERP0140
15.    C----------------------------------------------------------------------TERP0150
16.         IF(NL-IL)97,98,99                                              TERP0160
17.    C    NOT ENOUGH ENTRIES IN TABLES FOR THIS ORDER INTERPOLATION       TERP0170
18.       97 IL=NL                                                         TERP0180
19.       98 L=1                                                           TERP0190
20.          GO TO 112                                                     TERP0200
21.       99 CONTINUE                                                      TERP0210
```

```
      IL2=IL/2                                                          TERP0220
      IADD=MOD(IL,2)                                                    TERP0230
C     CHECK IF TABLES IN INCREASING OR DECREASING SEQUENCE              TERP0240
      IF(X(1)-X(NL))100,100,101                                         TERP0250
C     INCREASING SEQUENCE                                               TERP0260
  100 ILOW=IL2+1                                                        TERP0270
      IHI=NL-IL2-IADD                                                   TERP0280
      IUSEL=1                                                           TERP0290
      IUSEH=NL-IL+1                                                     TERP0300
      IBEG=ILOW+1                                                       TERP0310
      IEND=IHI-1                                                        TERP0320
      LAST=IEND-IL2+1                                                   TERP0330
      IADD=0                                                            TERP0340
      GO TO 102                                                         TERP0350
C     DECREASING SEQUENCE                                               TERP0360
  101 ILOW=NL-IL2                                                       TERP0370
      IHI=IL2+IADD+1                                                    TERP0380
      IUSEL=NL-IL+1                                                     TERP0390
      IUSEH=1                                                           TERP0400
      IBEG=IHI+1                                                        TERP0410
      IEND=ILOW-1                                                       TERP0420
      LAST=2                                                            TERP0430
      IADD=1-IADD                                                       TERP0440
C     CHECKS IF ARG IS SMALLER THAN TABLE VALUES                        TERP0450
  102 IF(ARG-X(ILOW))103,104,105                                        TERP0460
```

```
C     SMALLER THAN SMALLEST TABLE VALUE                          TERP0470
  103 L=IUSEL                                                    TERP0480
      GO TO 112                                                  TERP0490
  104 TERP=Y(ILOW)                                               TERP0500
      GO TO 117                                                  TERP0510
C     CHECKS IF ARG IS GREATER THAN TABLE VALUES                 TERP0520
  105 IF(X(IHI)-ARG)106,107,108                                  TERP0530
C     ARG GREATER THAN TABLE VALUE                               TERP0540
  106 L=IUSEH                                                    TERP0550
      GO TO 112                                                  TERP0560
  107 TERP=Y(IHI)                                                TERP0570
      GO TO 117                                                  TERP0580
C     SEARCHES X ARRAY TO BRACKET ARG                            TERP0590
  108 DO 109 N=IBEG,IEND                                         TERP0600
      IF(IUSEL-1)1080,1080,1081                                  TERP0610
 1080 M=N                                                        TERP0620
      GO TO 1082                                                 TERP0630
 1081 M=NL-N+1                                                   TERP0640
 1082 IF(X(M)-ARG)109,110,111                                    TERP0650
  109 CONTINUE                                                   TERP0660
      L=LAST                                                     TERP0670
      GO TO 112                                                  TERP0680
C     EQUALS ARGUMENT, RETURN OK                                 TERP0690
  110 TERP=Y(M)                                                  TERP0700
      GO TO 117                                                  TERP0710
```

```
      EUREKA                                                    TERP0720
  111 L=M-IL2+IADD                                              TERP0730
  112 CONTINUE                                                  TERP0740
C     INTERPOLATION SECTION                                     TERP0750
      SUM=0.0                                                   TERP0760
      DO 115 I=1,IL                                             TERP0770
      P=1.0                                                     TERP0780
      PK=1.0                                                    TERP0790
      IN=L+I-1                                                  TERP0800
      DO 114 IP=1,IL                                            TERP0810
      IF(IP-I)113,114,113                                       TERP0820
  113 INP=L+IP-1                                                TERP0830
      P=P*(ARG-X(INP))                                          TERP0840
      PK=PK*(X(IN)-X(INP))                                      TERP0850
  114 CONTINUE                                                  TERP0860
      SUM=SUM+P*Y(IN)/PK                                        TERP0870
  115 CONTINUE                                                  TERP0880
      TERP=SUM                                                  TERP0890
  117 RETURN                                                    TERP0900
      END                                                       TERP0910
END OF LISTING.     0 *DIAGNOSTIC* MESSAGE(S).
```

## 10. OTHER COMPLEMENTARY ACTIVITIES

To promote a vigorous exchange of information on electron scattering between the theoretical and experimental communities, a city-wide series of colloquia was initiated with the support of Gulf General Atomic. The series has been known as CAMP (Colloquia on Atomic and Molecular Processes). During the contract period, the following CAMP colloquia have been of interest to this program:

| | |
|---|---|
| March 8, 1967 | "Energetic Ions from Diatomic Molecules," Dr. Lee J. Keiffer, Joint Institute for Lab Astrophysics, University of Colorado, Boulder, Colorado |
| March 14, 1967 | "Theory of Near Adiabatic Collisional Transitions," Professor K. M. Watson, University of California, Berkeley, Physics Department |
| March 31, 1967 | "Atomic Scattering Spectroscopy: Analysis of Scattering of $He^+$ by Ne and Ar," Dr. Felix T. Smith, Stanford Research Institute, Menlo Park, California |
| April 28, 1967 | "Total Elastic and Inelastic Heavy Particle Collisions in the Energy Range 10 to 1000 eV. A: Elastic Scattering in the Alkali-Rare Gas System; B: Ionization Due to Rare Gas Metastable Collisions," Dr. Manfred Hollstein, Stanford Research Institute, Menlo Park, California |
| May 4, 1967 | "The Importance of Polarization in Low Energy Electron Molecular Collisions - An Application to $H_2$," Dr. Neil F. Lane, Department of Physics, Rice University, Houston, Texas |
| October 16, 1967 | "The Excitation and Spectroscopy of H-like Atoms," Dr. Hans Kleinpoppen, Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado |
| November 3, 1967 | "Low Energy Rotational Excitation Cross Sections Derived from Spectroscopic Data," Dr. Marvin Mittleman, Space Science Laboratory, University of California, Berkeley, California |

| | |
|---|---|
| December 11, 1967 | "Proton H-Atom Collisions," Professor M. R. C. McDowell, Goddard Space Flight Center, Greenbelt, Maryland |
| April 4, 1968 | "Ionization Processes of Molecules at Low Energies," Professor R. Stephen Berry, Department of Chemistry, University of Chicago, Chicago, Illinois |
| May 17, 1968 | "Polarization of Scattered Electrons," Professor E. Reichart, Department of Physics, University of Mainz, Mainz, Germany |

Probably the most significant activity this year was the Working Session on Electron H-Atom Collisions. The text of the notice and the program for the meeting are presented below.

## WORKING SESSION ON ELECTRON H-ATOM COLLISIONS

The detailed experimental and theoretical study of electron hydrogen atom collisions has developed to the point where our group at Gulf General Atomic, in conjunction with the group at the University of California, San Diego, plan to spend two days in a "working session" in order to examine what has been done, what is being done, and what can be done to most effectively study (e-H) collisions. The days we have in mind are Monday and Tuesday, April 8 and 9.

In particular, we plan to examine resonance and threshold problems since these areas have received the most extensive study of late. We have invited R. Damburg and A. Temkin to help organize discussion during our first day and to give colloquia on topics of particular interest. We plan to have several other talks by J. C. Y. Chen and ourselves, but for the most part our program will be informal and will stress the broadest possible exchange of ideas. We hope to spend one day together in an informal meeting while the second day (or part of the day) we are setting aside for the exchange of thoughts on a more individual basis. This will occur both here and at the University.

For those who would like to join us, arrangements will be made at a local hotel. We plan to get together for dinner Monday evening. Since time is already short, from those who will join us, we would appreciate word as soon as possible.

J. William McGowan
James F. Williams
GULF GENERAL ATOMIC

WORKSHOP ON ELECTRON HYDROGEN-ATOM COLLISIONS

Monday, April 8, 1968

| | | |
|---|---|---|
| AM SESSION: | La Salle Room, La Jolla Beach & Tennis Club | |
| 9:00 - 9:30 | Business and Coffee | |
| 9:30 - 12:30 | Elastic and Inelastic Electron Scattering | |
| | Chairman: Edward Gerjuoy | |
| | Review Experimental Measurements | J. William McGowan<br>Atomic Physics Lab<br>Gulf General Atomic |
| | Excitation of the Hydrogen Atom by Electron Impact | R. Damburg<br>Latvian Academy of Science |
| | Solutions of the Faddeev Equation for the (e-H) System | J. C. Y. Chen<br>University of California<br>San Diego |
| Lunch<br>12:30 - 1:45 | Scripps Institute of Oceanography<br>Cafeteria<br>After lunch, a visit to Scripps Physiological Research Lab | |
| PM SESSION:<br>2:00 - 5:00 | IGPP Building, University of California, San Diego<br>Ionization Threshold Studies | |
| | Chairman: Kenneth M. Watson | |
| | Black Box Aspects of the Threshold Law for Ionization | G. H. Wannier<br>University of Oregon |
| 3:30 | Coffee Break | |
| | An Approach to the Electron Atom Ionization Threshold Behavior | A. Temkin<br>NASA-Goddard Space Flight Center |
| Evening: | La Valencia Hotel | |
| | Cocktail hour at 7:00<br>Dinner at 8:00 | |

WORKSHOP ON ELECTRON HYDROGEN-ATOM COLLISIONS

Tuesday, April 9, 1968

| | |
|---|---|
| AM SESSION: | La Salle Room, La Jolla Beach & Tennis Club |
| 9:00 - 12:00 | Joint Experimental and Theoretical Workshop |
| | Chairman: Marvin Mittleman |
| | Possible Topics: |
| | Polarization of Radiation |
| | Polarized Electron and Atom Beams |
| | Coincidence Experiments |
| | Angular Correlation Experiments |
| | The Application of Born Approximation |
| | Lorentz Decay |
| | Removal of Degeneracy |
| | Definition of Threshold |
| | Cascade of Radiation |
| | Potential Resonances |
| 12:00 | Lunch at La Jolla Beach & Tennis Club Dining Room |
| PM SESSION: | IGPP Building, University of California, San Diego |
| 2:00 | Special Working Sessions |
| | Visits to Gulf General Atomic and the University of California, San Diego |
| NOTE: | At 11:00 a.m. at Gulf General Atomic Professor Gregory H. Wannier will be speaking on "Stark Ladders in Solids?" |

## REFERENCES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2. Burke, P. G., S. Ormonde, and W. Whitaker, "Low-Energy Electron Scattering by Atomic Hydrogen. I. The Close-Coupling Approximation," Proc. Phys. Soc. London 92, 319 (1967).

3. Chamberlain, G. E., S. J. Smith, and D. W. O. Heddle, "Excitation of the 2p State of Hydrogen by Electrons of Near Threshold Energy," Phys. Rev. Letters 12, 647 (1964).

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# APPENDIX I

## ABSTRACTS OF PAPERS GIVEN AT SCIENTIFIC MEETINGS

# LYMAN-ALPHA PRODUCTION AND POLARIZATION IN $He^+$ COLLISIONS WITH H AND $H_2$*

Robin A. Young, R. F. Stebbings,† and J. Wm. McGowan

Presented at 20th Annual Gaseous Electronics Conference of the American Physical Society, San Francisco, October 1967.

Measurements of the Lyman-alpha production from $He^+ + H(1s) \rightarrow He^+ + H(2p)$ collisions have been obtained over the energy range from 0.5 to 30 keV. At the lower ion energies the cross section remains large; this fact reflects the rotational interaction betv een states of the collision complex $HeH^+$. A similar result had been reported by Stebbings et al.[1] for the $H^+$-H collision system. Also presented are measurements of the total cross section for Lyman-alpha production from $He^+$-$H_2$ collisions. Some values of the polarization have been obtained for emission of Lyman-alpha from the collisions of $He^+$, $Ne^+$, and $Ar^+$ with atomic hydrogen.

*Work supported by the National Aeronautics and Space Administration, Goddard Space Flight Center, Contract NAS 5-11025.

†On leave from University College London, London, England.

1. R. F. Stebbings, R. A. Young, C. L. Oxley, and H. Ehrhardt, Phys. Rev. 138, A1312 (1965).

# THRESHOLD BEHAVIOR OF ELECTRON EXCITATION FUNCTIONS IN ATOMIC HYDROGEN*

J. F. Williams, E. K. Curley, and J. Wm. McGowan

Presented at 20th Annual Gaseous Electronics Conference of the American Physical Society, San Francisco, October 1967.

The excitation function, for electron impact, of the (1s - 2p) transition in atomic hydrogen appears to be finite at the threshold. When electron energy distribution functions of from 240 to 100 meV (FWHM) are unfolded from the observed Lyman-alpha radiation versus electron energy curve, it appears that the excitation function reaches a significant value within several tens of meV of the threshold and then drops sharply to about 60% of its peak threshold value. A report is given of attempts made to observe the resonance in the 2p excitation function, which is predicted by Burke et al. (1) to appear just below the n = 3 level.

*Work supported by the National Aeronautics and Space Administration, Goddard Space Flight Center, Contract NAS-5-11025.

1. P. G. Burke, S. Ormonde, and W. Whitaker, Phys. Rev. Letters 17, 800 (1966).

# (e-H) COMPOUND STATES REFLECTED IN THE H(2p) CHANNEL IN THE VICINITY OF n = 3*

J. William McGowan and James F. Williams

Presented at American Physical Society Meeting,
Los Alamos Scientific Laboratory, June 1968.

High resolution electron impact studies of the 2p excitation cross section of atomic hydrogen have been made in the vicinity of n = 3. Prominent resonance structure has been observed below and above n = 3. The structure below n = 3 qualitatively is in agreement with the predictions of Burke et al., [1] but in detail there is some difference as to the breadth of the (e-H) resonances. Above n = 3 there is evidence that a shape resonance is present.

*Work supported by the National Aeronautics and Space Administration, Goddard Space Flight Center, Contract NAS-5-11025.

[1] P. G. Burke, S. Ormonde, and W. Whitaker, Proc. Phys. Soc. 92, 319 (1967).

# COMPARISON OF THE CALCULATED AND OBSERVED RESONANCES IN THE (e-H) ELASTIC SCATTERING CHANNEL ABOVE 10.0 eV*

J. William McGowan and S. Ormonde†

Submitted to the Arnold Sommerfeld Centennial Memorial Meeting and International Symposium on the Physics of One and Two Electron Atoms, Munich, September 1968.

Recent measurements of the electron hydrogen atom elastic scattering cross section show a rather wide structure immediately below the n = 2 threshold.(1) This structure has been attributed to the $^1D$ and $^3S$ compound states of $H^-$, which have already been partially discussed in the literature.(2-4) Since the observed effect of these states on the differential cross section appears to be considerably larger than expected from what we know of the resonances in the $^1S$ series, it was decided to compare the experiment with the results of a detailed close-coupling calculation of the resonances just below the n = 2 threshold. Preliminary results for the $^1D$ resonance place it at an energy of 10.15 eV with width $\Gamma$ = 0.0073 eV. When the energy distribution of the electron beam is folded into the calculated cross section, the agreement between theory and experiment is reasonably good. The effects of including higher hydrogenic states as well as taking into account the considerations of Damberg and Geltman(5) are presently being examined.

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†Quantum Systems, Incorporated, Albuquerque, New Mexico.

1. J. William McGowan, E. M. Clarke, and E. K. Curley, Phys. Rev. Letters 15, 917 (1965); 17, 66E (1966).
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# A DETAILED COMPARISON OF THE THEORETICAL AND EXPERIMENTAL RESULTS FOR THE 2p ELECTRON-IMPACT EXCITATION CROSS SECTION OF HYDROGEN*

J. William McGowan and J. F. Williams

Submitted to the Arnold Sommerfeld Centennial Memorial Meeting and International Symposium on the Physics of One and Two Electron Atom, Munich, September 1968.

At first glance one is satisfied with the agreement between theory and experiment in the threshold region of the 2p electron-impact excitation cross section of atomic hydrogen. However, when a detailed comparison is made in the region between the onset of the n = 2 level and the n = 4 level, one finds that there is much yet to be done with the theory. The measured value for the total cross section lies below the best theoretical value. For example, if we consider the interval between 0.2 and 1.5 eV above threshold, the measured cross section is only 80% of the value estimated by the correlation method.[1] Similar agreement between theory and experiment for 2s excitation was recently reported by Fite et al.[2] The shape resonance predicted in the $^1P$ channel just above threshold and the finite threshold of excitation are approximately the magnitude suggested by the theory. However, following the first shape resonance are at least two other small structures which appear to be real and which may be part of a series of such shape resonances. Unfortunately, the calculations that have been performed thus far have not been done on a fine enough grid to identify in which channel these other resonances lie.

As predicted by the six-state approximation,[3] there are a number of resonances just below the onset of the n = 3 level. However, there is not good agreement between the theoretically predicted and the measured resonances. Provided the positions that have been predicted are correct, one is lead to the conclusion that the dominant resonance structure is in the $^1P$ channel while less prominent structure appears in the $^1S$ channel. The theory, however, predicts that the principle resonance will be in the $^1D$ channel.

In our experimental results one of the most prominent features appears at the threshold of n = 3. This no doubt reflects a large shape resonance at the threshold of the n = 3 level. Part of the flux from this resonance will appear directly in the 2p channel while another portion of it will arrive

*Work supported by the National Aeronautics and Space Administration, Contract NAS 5-11025, and by Gulf General Atomic Incorporated private research funds.

there through cascade from the 3s and 3d states of the atom. Although detailed measurements of the resonance structure between n = 3 and n = 4 have not been completed, it is clear from our crude measurements that some measurable resonance structure does exist in this interval. One would hope that the calculations similar to those of Damburg and Geltman[4] will eventually be able to correct for the incompleteness in the original close-coupling approximation calculations.


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# APPENDIX II

## PAPERS RESULTING THIS YEAR FROM THE PROGRAM

# Faddeev Equations for Atomic Problems and Solutions for the ($e$,H) System*

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(Received 1 April 1968)

Solutions of the Faddeev equations for Coulomb potentials are investigated. A method which is of practical use for solving the Faddeev equations below the three-particle breakup threshold is developed. As an example, the method is applied to the (e, H) system in which the $H^-$ bound state and the lowest members of the resonances in both the singlet and the triplet $J = 0$ series are calculated. The results are in good agreement with the experimental measurements and previous calculations which used conventional methods.

## I. INTRODUCTION

The nonrelativistic three-body problem with two-body interactions has been formulated by Faddeev[1,2] in a way that allows straightforward computations. For short-range forces, the Faddeev equations have been applied successfully to a number of problems.[3-13] It is the purpose of this paper to show that the Faddeev equations are equally applicable to atomic problems as long as the total energy is below the three-body breakup threshold – for example, the calculation of three-body bound states and resonance energies and wave functions below the ionization energy. The significant advantage of the Faddeev equation over conventional methods is that the wave functions are calculated systematically along with the energy levels. No trial wave function is needed in the computation. Although this paper only contains a few illustrative examples all dealing with the $e$-H problem, we believe that the Faddeev equation has a considerably wider range of applicability. A brief account of this work was presented recently at the Leningrad Conference.[14]

In Sec. II, we give a simple derivation of the Faddeev equation, and review the method of reduction with respect to angular momentum. The method of solution is presented in Sec. III and applied to the $H^-$ problem in Sec. IV. A discussion of possible extensions is given in Sec. V.

## II. THE FADDEEV EQUATIONS

### A. Formal Derivation

The scattering matrix $T(s)$ for the three-particle system with two-body interactions is a solution of the equation

$$T(s) = V + VG_0(s)T(s), \tag{2.1}$$

$$\text{with } V = \sum_i V_i (V_i \equiv V_{jk}), \tag{2.2}$$

$$G_0(s) = (s - H_0)^{-1}, \tag{2.3}$$

where the three particles are labeled by $i$, $j$, and $k$, and $G_0(s)$ is the free three-particle Green's function. The "off-shell" scattering matrix $T_i(s)$ arising from the two-body potential $V_i$ above is given by the Lippmann-Schwinger equation

$$T_i(s) = V_i + V_i G_0(s) T_i(s). \tag{2.4}$$

Since $V_i$ acts only on two particles, the third particle is therefore left as a spectator in Eq. (2.4). Equation (2.4), in effect, is equivalent to the equation for two-particle scattering matrix; the presence of the spectator particle gives rise to merely a shift in the energy scale.

Now we decompose the three-particle scattering matrix $T(s)$ into three components

$$T(s) = T^{(1)}(s) + T^{(2)}(s) + T^{(3)}(s), \tag{2.5}$$

where $$T^{(i)}(s) = V_i + V_i G_0(s) T(s) . \tag{2.6}$$

As it stands, Eq. (2.6) is a set of integral equations with each $T^{(i)}$ coupled to all three operators $T^{(j)}$, $j = 1$, 2, and 3. The main difference between these equations and the Faddeev equations is that, in the latter, each $T^{(i)}$ is only coupled to two $T^{(j)}$'s with $j \neq i$, and as a result, the kernel of the integral equation is less singular. We give here a simple derivation of the Faddeev equations:

Define the expression

$$\Omega = T^{(i)}(s) - T_i(s) - \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s). \tag{2.7}$$

One can readily show by utilizing Eqs. (2.4)–(2.6) that

$$\Omega = V_i + \sum_{j=1}^{3} V_i G_0 T^{(j)} - V_i - V_i G_0 T_i - \sum_{j \neq i}^{3} V_i G_0 T^{(j)} - \sum_{j \neq i}^{3} V_i G_0 T_i G_0 T^{(j)} = V_i G_0 \Omega. \tag{2.8}$$

Since $V_i G_0(s)$ is not the identity operator, Eq. (2.8) implies that $\Omega = 0$ for each $i$. We then obtain for $T^{(i)}(s)$ the equations

$$T^{(i)}(s) = T_i(s) + \sum_{j \neq i} T_i(s) G_0(s) T^{(j)}(s), \quad i = 1, 2, 3, \tag{2.9}$$

which are the well-known Faddeev equations.[1] In the matrix form:

$$\begin{pmatrix} T^{(1)}(s) \\ T^{(2)}(s) \\ T^{(3)}(s) \end{pmatrix} = \begin{pmatrix} T_1(s) \\ T_2(s) \\ T_3(s) \end{pmatrix} + \begin{pmatrix} 0 & T_1(s) & T_1(s) \\ T_2(s) & 0 & T_2(s) \\ T_3(s) & T_3(s) & 0 \end{pmatrix} G_0(s) \begin{pmatrix} T^{(1)}(s) \\ T^{(2)}(s) \\ T^{(3)}(s) \end{pmatrix}. \tag{2.10}$$

This is a coupled set of integral equations in five variables. Since no approximation is made on this formal transformation, the solution of Eq. (2.10) yields $T^{(1)}$, $T^{(2)}$, and $T^{(3)}$ whose sum is the exact solution of the original equation (2.1).

The Faddeev equations can also be interpreted diagrammatically. Let us represent $T_1$ by the sum of the diagrams as shown in Fig. 1 and similarly for $T_2$ and $T_3$. For the $T$'s with a superscript, we use the symbols shown in Fig. 2. The Faddeev equations are then given by Fig. 3. One can easily see that the iterative solution of the three equations in Fig. 3 using the equation in Fig. 1 reproduces all the diagrams in perturbation theory. Our formal derivation given earlier simply shows that the Eqs. in Fig. 3 are valid even if the perturbation series fails to converge. In the diagrammatic representation, it is physically evident that $T^{(1)}$ is that part of the full three-body $T$ matrix where particles 2 and 3 undergo a final-state interaction. Since $T_i$ already represent a complete sequence of two-body interactions, each $T^{(i)}$ can only couple to $T^{(j)}$, $j \neq i$. As mentioned earlier, this decoupling of $T^{(i)}$ from itself results in a less singular kernel as compared to the original equation (2.6). This is due to the fact that each $T_i$ is associated with a $\delta$ function corresponding to the momentum conservation of the $i$th particle, and the decoupling removes the repeated $\delta$ functions.

### B. Three-Body Kinematics

To reduce the Faddeev equations, a suitable set of basis variables must first be chosen. For this purpose, the momentum representation is adopted. Let the masses and asymptotic momenta of the three particles be denoted by $m_1$, $m_2$, and $m_3$, and $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$, respectively. An appropriate set of basis variables may be constructed by taking certain combinations of the momenta in the center-of-mass system of the three particles. For $T^{(1)}$, the suitable basis variables are the pair of independent momentum

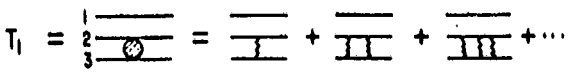

FIG. 1 Diagrams for the two-body scattering matrix $T_i$. The wavy lines represent the two-particle potential $V_i$.

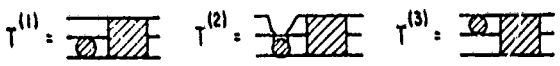

FIG. 2 Symbols representing the three-body scattering matrix $T^{(i)}$ with a pair of particles undergoes a final-state interaction.

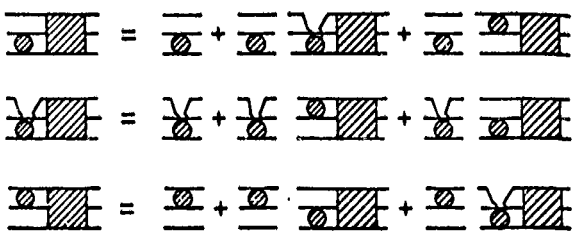

FIG. 3 Diagrammatical representation of the Faddeev equations. The gap between two diagrams represents a a noninteracting three-body Green's function.

variables.[3]

$$\vec{p}_1=[m_3\vec{k}_2-m_2\vec{k}_3]/[2m_2m_3(m_2+m_3)]^{1/2}\,,\quad \vec{q}_1=[m_1(\vec{k}_2+\vec{k}_3)-(m_2+m_3)\vec{k}_1]/[2m_1(m_2+m_3)(m_1+m_2+m_3)]^{1/2}, \tag{2.11}$$

and their conjugated pairs $\vec{p}_2\vec{q}_2$ and $\vec{p}_3\vec{q}_3$ which are obtained by a cyclic interchange of subscripts in Eqs. (2.11) are the appropriate sets for $T^{(2)}$ and $T^{(3)}$ respectively.

The nonrelativistic kinetic energy in the center-of-mass frame may be written in any pair of basis variables;

$$H_0=p_1^2+q_1^2=p_2^2+q_2^2=p_3^2+q_3^2\,. \tag{2.12}$$

Consequently, the corresponding state vector $|\vec{k}_1\vec{k}_2\vec{k}_3\rangle$ may be represented in several equivalent forms

$$|\vec{k}_1\vec{k}_2\vec{k}_3\rangle=|\vec{p}_1\vec{q}_1\rangle_1=|\vec{p}_2\vec{q}_2\rangle_2=|p_3q_3\rangle_3\,, \tag{2.13}$$

where the extra subscript keeps track of the proper pair of basis variables.

These sets of basis momentum variables are linearly dependent on each other. The relations are summarized below.

$$\vec{p}_1=\alpha_{12}\vec{p}_2-\beta_{12}\vec{q}_2=-\alpha_{13}\vec{p}_3+\beta_{13}\vec{q}_3\,,\quad \vec{q}_1=\beta_{12}\vec{p}_2-\alpha_{12}\vec{q}_2=-\beta_{13}\vec{p}_3-\alpha_{13}\vec{q}_3\,, \tag{2.14a}$$

$$\vec{p}_2=-\alpha_{21}\vec{p}_1+\beta_{21}\vec{q}_1=-\alpha_{23}\vec{p}_3-\beta_{23}\vec{q}_3\,,\quad \vec{q}_2=-\beta_{21}\vec{p}_1-\alpha_{21}\vec{q}_1=\beta_{23}\vec{p}_3-\alpha_{23}\vec{q}_3\,, \tag{2.14b}$$

$$\vec{p}_3=-\alpha_{32}\vec{p}_2+\beta_{32}\vec{q}_2=-\alpha_{31}\vec{p}_1-\beta_{31}\vec{q}_1\,,\quad \vec{q}_3=-\beta_{32}\vec{p}_2-\alpha_{32}\vec{q}_2=\beta_{31}\vec{p}_1-\alpha_{31}\vec{q}_1\,, \tag{2.14c}$$

where $\alpha_{ij}\equiv[m_im_j/(m_i+m_k)(m_j+m_k)]^{1/2}$, $\beta_{ij}\equiv(1-\alpha_{ij}^2)^{1/2}$ (2.15)

We will frequently interchange these basis momentum variables among different sets for convenience.

### C. Separation of Angular Momentum

A separation of the angular momentum states in the Faddeev equations can be carried out using the relative angular momentum of two particles, which is combined with the angular momentum of the third particle in the over-all center-of-mass system.[8,15] In this decoupling scheme, the state vector $[\vec{p}_i,\vec{q}_i\rangle_i$ may be expanded in terms of a set of orthonormal partial-wave states $|p_i l m_l,\ q_i L m_L\rangle_i$. Since the total angular momentum $J$ is conserved, we may in general consider the states to be diagonal in $J$. These states are given by

$$|pqJMlL\rangle_i=(-)^{L-l-M}(2J+1)^{\frac{1}{2}}\sum_{m_lm_L}\begin{pmatrix}J & l & L\\ -M & m_l & m_L\end{pmatrix}|plm_l,qLm_L\rangle_i\,, \tag{2.16}$$

with

$$|plm_l,qLm_L\rangle_i=Y_{lm_l}(\hat{p})Y_{Lm_L}(\hat{q})|\vec{p},\vec{q}\rangle_i\,, \tag{2.17}$$

$${}_i\langle plm_l,qLm_L|p'l'm_{l'},q'L'm_{L'}\rangle_i=(pq)^{-2}\delta(p-p')\,\delta(q-q')\,\delta_{ll'}\,\delta_{LL'}\,\delta_{m_lm_{l'}}\,\delta_{m_Lm_{L'}}\,, \tag{2.18}$$

where the Wigner 3$j$ symbol is adopted for the Clebsch-Gordan coefficients.

The Faddeev equations [Eqs. (2.9)] may be written in this representation as

$$\Psi_\alpha^{(i)}(p;q;s) = \Phi_\alpha^{(i)}(p,q,s) + \tfrac{1}{4}\sum_{\alpha_j}\sum_{j\neq i}\int_0^\infty dp_j{}^2\int_0^\infty dq_j{}^2\,\mathcal{K}_j^{(i)}(pq\alpha|p_jq_j\alpha_j)[p_jq_j/(p_j{}^2+q_j{}^2-s)]$$

$$\times\Psi_{\alpha_j}^{(j)}(p_j,q_j,s), \tag{2.19}$$

$$\text{with}\quad \Psi_\alpha^{(i)}(p,q,s) \equiv {}_i\langle pq\alpha|T^{(i)}(s)|\vec{k}_1\vec{k}_2\vec{k}_3\rangle, \tag{2.20}$$

$$\Phi_\alpha^{(i)}(p,q,s) \equiv {}_i\langle pq\alpha|T_i(s)|\vec{k}_1\vec{k}_2\vec{k}_3\rangle, \tag{2.21}$$

$$\mathcal{K}_j^{(i)}(pq\alpha|p_jq_j\alpha_j) \equiv {}_i\langle pq\alpha|T_i(s)|p_jq_j\alpha_j\rangle_j, \tag{2.22}$$

where for convenience the discrete quantum numbers ($JMlL$) are collectively denoted by $\alpha$. The physical interpretation of the equations is straightforward. The quantity $\Psi_{\alpha_j}^{(i)}(p_jq_js)$ represents the contribution to the three-particle scattering amplitude in which particles $j$ and $k(j\neq k\neq i)$ undergo final-state interaction with relative angular momentum $l_j$. The quantity $\Phi_{\alpha_i}^{(i)}(p_jq_js)$ represents the scattering amplitude in which particle $i$ acts as a spectator. The initial state which is denoted by $|\vec{k}_1\vec{k}_2\vec{k}_3\rangle$ is arbitrary. The quantity $p$ is proportional to the magnitude of the relative momentum between particles $j$ and $k$, and the quantity $q$ is proportional to the magnitude of the momentum of particle $i$ in the three-particle center-of-mass frame.

Utilizing Eqs. (2.16)–(2.18), we obtain for the kernel $\mathcal{K}_j^{(i)}$ [defined in Eq. (2.22)] the expression

$$\mathcal{K}_j^{(i)}(pq\alpha|p_jq_j\alpha_j) = (-)^{L+L'-l-l'}\sum_{\substack{m_lm_L\\m_{l'}m_{L'}}}\begin{pmatrix}J & l & L\\ -M & m_l & m_L\end{pmatrix}\begin{pmatrix}J & l' & L'\\ -M & m_{l'} & m_{L'}\end{pmatrix}$$

$$\times\int d\hat{p}_j\,d\hat{q}_j\,d\hat{p}_i\,d\hat{q}_i\;{}_i\langle\vec{p}\vec{q}|T_i(s)|\vec{p}_j\vec{q}_j\rangle_j\,(2J+1)Y_{lm_l}^*(\hat{p}_i)Y_{Lm_L}^*(\hat{q}_i)Y_{l'm_{l'}}(\hat{p}_j)$$

$$\times Y_{L'm_{L'}}(\hat{q}_j). \tag{2.23}$$

Since $T_i$ involves only two-body potential $V_i$ [see Eq. (2.4)], the matrix element ${}_i\langle\vec{p}\vec{q}|T_i(s)|\vec{p}_j\vec{q}_j\rangle_j$ in Eq. (2.23) may be reduced to a two-particle matrix element. According to Eqs. (2.3), (2.12), and (2.13), we have

$${}_i\langle\vec{p}\vec{q}\,|T_i(s)|\vec{p}_j\vec{q}_j\rangle_j = {}_i\langle\vec{p}\vec{q}\,|T_i(s)|p_iq_i\rangle_i = \delta(\vec{q}-\vec{q}_i)\langle\vec{p}\,|\tilde{T}_i(s-q^2)|\vec{p}_i\rangle, \tag{2.24}$$

$$\text{with}\quad \delta(\vec{q}-\vec{q}_i) = 2q^{-1}\delta(q^2-q_i^2)\,\delta(\cos\theta_{\vec{q}}-\cos\theta_{\vec{q}_i})\,\delta(\varphi_{\vec{q}}-\varphi_{\vec{q}_i}), \tag{2.25}$$

where $\tilde{T}_i$ is the two-particle scattering matrix in the Hilbert space of the two-particle states. We may make use of the decomposition

$$\langle\vec{p}\,|\tilde{T}_i(s-q^2)|\vec{p}_i\rangle = -\frac{1}{2\pi^2}\sum_{l=0}^{\infty}(2l+1)\,P_l(\cos\theta_{\vec{p}\vec{p}_i})\,t_l^{(i)}(p,p_i;s-q^2), \tag{2.26}$$

where the scattering amplitude between particles $j$ and $k$ with angular momentum $l$ is normalized according to the equation

$$t_l^{(i)}(p,p;p^2) = e^{i\delta_l}(\sin\delta_l)/p. \tag{2.27}$$

Here $p^2$ is the two-body center-of-mass energy.

When Eqs. (2.24)–(2.26) are utilized, the kernel in the Faddeev equations may be written as[8]

$$\mathcal{K}_j^{(i)}(pq\alpha|p_jq_j\alpha_j) = \int_{-1}^{1}d\cos\theta_{\vec{q}_j\vec{p}_j}\,A_{\alpha\alpha_j}(\theta_{\vec{p}_i\vec{p}_j},\theta_{\vec{q}_i\vec{p}_j},\theta_{\vec{q}_j\vec{p}_j})\,\delta(q^2-q_i^2)t_l^{(i)}(p,p_i;s-q^2) \tag{2.28}$$

$$\text{with } A_{\alpha\alpha'}(\theta_{\vec{q}_j\vec{p}_j}) = \frac{(-)^{L+L'-l-l'+1}}{q} 16\pi^{\frac{1}{2}}(2l'+1)^{\frac{1}{2}}\delta_{JJ'}\delta_{MM'} \sum_{\bar{m}_l\bar{m}_L\bar{m}_{L'}} \begin{pmatrix} l & L & J \\ m_l & m_L & -m_{L'} \end{pmatrix}\begin{pmatrix} l' & L' & J' \\ 0 & \bar{m}_{L'} & -\bar{m}_{L'} \end{pmatrix}$$

$$\times Y^*_{l\bar{m}_l}(\theta_{\vec{p}_i\vec{p}_j},0)Y^*_{L\bar{m}_L}(\theta_{\vec{q}_i\vec{p}_j},0)Y_{L'\bar{m}_{L'}}(\theta_{\vec{q}_j\vec{p}_j},0), \tag{2.29}$$

where $\theta_{\vec{q}_j\vec{p}_j}$, for example, is the angle between momentum variables $\vec{q}_j$ and $\vec{p}_j$. It should be noted that these angles are related through the relations between different sets of pair momentum variables [see Eqs. (2.14)].

The above result was derived for any angular momentum state $J$ of the three-particle system. For convenience, we will consider explicitly only states corresponding to zero total angular momentum. For this $J=0$ case, $\alpha=(00ll)\equiv l$, and Eq. (2.29) becomes

$$A_{ll'}(\theta_{\vec{q}_j\vec{p}_j}) = \frac{2(-)^{l+l'}}{\pi q}(2l+1)^{\frac{1}{2}}(2l'+1)^{\frac{1}{2}}p_l(\cos\theta_{\vec{q}_i\vec{p}_i})p_{l'}(\cos\theta_{\vec{q}_j\vec{p}_j}), \tag{2.30}$$

with $p_i^2 = p_j^2 + q_j^2 - q^2$ and

$$\cos\theta_{\vec{q}_i\vec{p}_i} = (ij)\frac{[\alpha_{ij}^2(q_j^2-q^2)+\beta_{ij}^2(a^2-p_j^2)]}{2\alpha_{ij}\beta_{ij}qp_i}, \tag{2.31}$$

$$\cos\theta_{\vec{p}_j\vec{q}_j} = (ij)\frac{[\beta_{ij}^2p_j^2+\alpha_{ij}^2q_j^2-q^2]}{2\alpha_{ij}\beta_{ij}p_jq_j}, \tag{2.32}$$

where $(ij)$ denotes that $(12)=(23)=(31)=1$ and $(21)=(32)=(13)=-1$.

Substituting Eq. (2.28) with $A_{ll'}$ given by Eq. (2.30) back into Eq. (2.19), and integrating over the angles, we obtain for the Faddeev equations

$$\Psi_l^{(i)}(p,q,s) = \Phi_l^{(i)}(p,q,s) + \sum_{j\neq i}\sum_{l'=0}\int_0^\infty dq_j^2\int_{L_{ij}}^{U_{ij}} dp_j^2 \times \frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_j\vec{q}_j})}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)} \times t_l^{(i)}(p,p_i;s-q^2)\Psi_{l'}^{(j)}(p_j,q_j,s), \quad i=1,2,3 \tag{2.33}$$

$$\text{with } U_{ij} = (\alpha_{ij}q_j+q)^2/\beta_{ij}^2, \quad L_{ij} = (\alpha_{ij}q_j-q)^2/\beta_{ij}^2. \tag{2.34}$$

It is clear that if $t_l^{(i)}(p,p_i;s-q^2)$ is expanded in a sum of terms separable in $p$ and $p_i$, then the $p$ dependence of $\Psi_l^{(i)}(p,q,s)$ becomes explicit ($p$ does not appear in the kinematic functions or the limits of integrations), and the coupled integral equations in two variables [Eq. (2.33)] can be reduced to equations of one variable.[10,12] We will consider the application of these equations to three-particle atomic systems in which the interaction proceeds through two-body Coulomb potentials between each pair of particles.

## III. THE METHOD OF SOLUTION

### A. Eigenfunction Expansion for "Off-Shell" Amplitude

As mentioned before, the partial-wave Faddeev equations of two variables may be reduced to equations of one variable if the "off-shell" two-body scattering amplitudes $t_l$ are represented in sums of separable terms. In general, if the two-body potentials $V_l^{(i)}$ for a system are given, the two-body amplitude $t_l^{(i)}$ can be obtained from the solution of the Lippmann-Schwinger equation

$$t_l^{(i)}(p,p';E) = V_l^{(i)}(p,p') + \pi^{-1}\int_0^\infty dp''\,p''V_l^{(i)}(p,p'')t_l^{(i)}(p'',p';E)/(p''^2-E). \tag{3.1}$$

Since the argument $E$ is replaced by $(s-q^2)$ in the Faddeev equations, it is negative-definite provided the three-particle energy $s$ is below the three-particle threshold ($s=0$). For negative values of $E$, the $(p''^2-E)^{-1}$ term in Eq. (3.1) is nonsingular, and it is well known that the solution for $t_l^{(i)}$ can be expressed

in terms of eigenfunctions of the homogeneous portion of Eq. (3.1).

The solution $\phi_{nl}^{(i)}$ of the homogeneous Lippmann-Schwinger equation and the corresponding eigenvalues $\lambda_{nl}^{(i)}$ are defined by

$$\lambda_{nl}^{(i)}(E)\phi_{nl}^{(i)}(p,E) = \pi^{-1}\int_0^\infty dp''^2\,[p''V^{(i)}(p,p'')/(p''^2 - E)]\,\phi_{nl}^{(i)}(p'',E), \tag{3.2}$$

with the orthonormality property

$$\pi^{-1}\int_0^\infty dp''^2\,p''\phi_{nl}^{(i)}(p'',E)\phi_{ml}^{(i)}(p'',E)/(p''^2 - E) = \delta_{nm}. \tag{3.3}$$

Since $\phi_{nl}^{(i)}$ constitutes a complete set, the two-body amplitude $t_l^{(i)}$ can be expanded in the form

$$t_l^{(i)}(p,p';E) = \sum_{n=0}^{\infty} C_{nl}^{(i)}(p',E)\phi_{nl}^{(i)}(p,E). \tag{3.4}$$

Substitution of (3.4) into Eq. (3.1) yields, with the help of Eqs. (3.2) and (3.3),

$$t_l^{(i)}(p,p';E) = \sum_{n=0}^{\infty} \{\lambda_{nl}^{(i)}(E)/[1-\lambda_{nl}^{(i)}(E)]\}\,\phi_{nl}^{(i)}(p,E)\,\phi_{nl}^{(i)}(p',E). \tag{3.5}$$

This is the desired representation for $t_l^{(i)}$ in the sums of separable terms.

In momentum representation, the Coulomb potential is

$$V_l^{(i)}(p,p') = -(Z_i\mu_i^{\frac{1}{2}}/\sqrt{2}\,pp')Q_l(p^2+p'^2)/2pp', \tag{3.6}$$

where the $Q_l$'s are the Legendre functions of the second kind, $\mu_i$ is the reduced mass, and $Z_i$ is the product of the charges (i.e., $Z_jZ_k$) of the two particles. For this potential the eigenfunction $\phi_{nl}^{(i)}$ and the eigenvalue $\lambda_{nl}^{(i)}$ are both known analytically.[16] We have

$$\phi_{nl}^{(i)}(p,E) = [N_{nl}(E)p^l/(p^2-E)^{l+1}]\,C_{n-l-1}^{\,l+1}[(p^2+E)/(p^2-E)], \quad n>l \tag{3.7}$$

and $$\lambda_{nl}^{(i)}(E) = -Z_i\mu_i^{\frac{1}{2}}/n\sqrt{-2E}, \tag{3.8}$$

where $n>l$ and the normalization constant is

$$N_{nl}(E) = [2^{4l+3}n(n-l-1)!/\Gamma(n+l+1)]^{\frac{1}{2}}\,l!\,(-E)^{(2l+3)/4}. \tag{3.9}$$

The $C_{m-1}^{\,l+1}(x)$'s in Eq. (3.7) are the Gegenhauer polynomials[17]

$$C_{m-1}^{l+1}(x) = \frac{\Gamma(m+2l+1)}{\Gamma(m)\Gamma(2l+2)}\,F\left(m+2l+1,1-m;l+\tfrac{3}{2};\tfrac{1}{2}(1-x)\right) = \sum_{\gamma=0}^{m-1} a_\gamma^{(l+1)}(m)\left(\frac{x-1}{2}^{\gamma}\right), \tag{3.10}$$

with $$a_\gamma^{(l+1)}(m) = [2(m+2l+\gamma)(m-\gamma)/\gamma(2l+2\gamma+1)]\,a_{\gamma-1}^{(l+1)}(m), \tag{3.11}$$

where the recursion relation for the $a$'s starts with

$$a_0^{(l+1)}(m) \equiv (m+2l)!/(2l+1)!\,(m-1)!. \tag{3.12}$$

### B. Coupled Single-Variable Integral Equations

Utilizing the separable representation [Eq. (3.5)] for the off-shell two-particle amplitude, the $p$ dependence of $\Psi_\alpha^{(i)}(p,q,s)$ can now be made explicit. Let us return to the Faddeev equations for total $J=0$. From Eq. (2.33), it is clear with the help of Eq. (3.5) that $\Psi_l^{(i)}(p,q,s)$ can be expressed as

$$\Psi_l^{(i)}(p,q,s) = \Phi_l^{(i)}(p,q,s) + \sum_n \{\lambda_{nl}^{(i)}\ (s-q^2)/[1-\lambda_{nl}^{(i)}(s-q^2)]\}\phi_{nl}^{(i)}\ (p,s-q^2)\chi_{nl}^{(i)}(q,s). \tag{3.13}$$

Substituting Eq. (3.13) into Eq. (2.33), we obtain a set of coupled single-variable integral equations for $\chi_{nl}^{(i)}(q,s)$:

$$\chi_{nl}^{(i)}(q,s)=\eta_{nl}^{(i)}(q,s)+\sum_{n',l';j\neq i}\int_0^\infty dq_j^{\,2}\,\mathcal{K}_{nl,nl'}^{(i,j)}(q,q_j;s)\chi_{n'l'}^{(j)}(q_j,s),\quad i=1,2,3 \tag{3.14}$$

with $$\eta_{nl}^{(i)}(q,s)=\sum_{l',j\neq i}\int_0^\infty dq_j^{\,2}\int_{L_{ij}}^{U_{ij}}dp_j^{\,2}\,\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_j\vec{q}_j})$$

$$\times\phi_{nl}^{(i)}(p_i,s-q^2)\phi_{l'}^{(j)}(p_j,q_j), \tag{3.15}$$

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j;s)=\int_{L_{ij}}^{U_{ij}}dp_j^{\,2}\,\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{\frac{1}{2}}P_l(\cos\theta_{\vec{p}_i\vec{q}_i})P_{l'}(\cos\theta_{\vec{p}_i\vec{q}_j})}{4\pi\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)[1-\lambda_{n'l'}^{(j)}(s-q_j^2)]}$$

$$\times\phi_{nl}^{(i)}(p_i,s-q^2)\lambda_{n'l'}^{(j)}(s-q_j^2)\phi_{n'l'}^{(j)}(P_j,s-q_j^2). \tag{3.16}$$

Equations (3.14) are the basic working equations. We will now examine their physical implications.

Let us first examine the singularities of the kernel $\mathcal{K}$ given by Eq. (2.16). For negative values of $s$, two-particle bound states of the system (if they exist) play an important role in the analytic structure of the kernel $\mathcal{K}$. Denote the two-particle bound-state energy by $-\epsilon$. For each such two-particle state, there is a corresponding eigenvalue $\lambda$ which equals to unity at $-\epsilon$. The denominator $1-\lambda_{n'l'}^{(j)}(s-q^2)$ in the kernel then vanishes at $q^2=s+\epsilon$ for $s>-\epsilon$, therefore creating a branch point for $\chi_{nl}^{(i)}(q,s)$ at $s=-\epsilon$. Three-particle bound states can only occur below the branch points. The region between the lowest and the next branch points is the energy region for purely elastic scattering of a particle by a two-particle system in its ground state. A single inelastic process occurs above the second threshold, and so forth. By solving the Faddeev equations, we can obtain bound-state and resonance energies and wave functions below the three-particle breakup threshold.

Now if there is no two-particle bound state between any pair of particles in the three-particle system, the behavior of the kernel $\mathcal{K}$ becomes less complicated, since in this case the kernel is pure real below $s=0$. Again, Eqs. (3.14) can be solved in a straightforward manner for both the energies and wave functions of any possible three-particle bound states.

It should be noted, however, that if the total energy $s$ is positive (i.e., above the three-particle breakup threshold), then there is a region $0<q^2<s$ where the two-particle energy $s-q^2$ is positive and the expansion for the off-shell two-particle amplitude [Eq. (3.5)] in general fails to converge. The method discussed above becomes unsuitable. This includes the problems of three-particle breakup such as, for example, the ionization of hydrogen atoms by electron impact.

We remark here that, for the Coulomb interaction, the two-body $T$ matrix $t_l(p,p',E)$ is singular at $p^2=E$, $p'^2=E$ or $p=p'$ for all $E$. The first two regions are inaccessible below the three-particle threshold (ionization energy), because $E$ is negative-definite while $p$ and $p'$ are positive. The region $p=p'$ is accessible but the kernel $\mathcal{K}_{nl,n'l'}(q,q_j;s)$ is already the result of an integration over $p_j^2$. Since the singularity at $p=p'$ is only logarithmatic, the kernel no longer contains such a logarithmatic singularity. This, we believe, is the reason why the three particle atomic problem can be handled by the Faddeev equations without further modification, as long as the total energy is below the three-particle breakup threshold.

So far the initial states of the three-particle system are left unspecified. This is possible because the kernel of the integral equation is independent of the initial state, and the energy spectrum of the three-body system is determined entirely by the kernel. The specification of the initial state and the corresponding inhomogeneous terms are, however, of importance for the wave function of the scattering problem. We now show how this term may be calculated.

For a physical scattering process, one usually has an initial state consisting of two interacting subsystems; in the present case, a particle plus a two-particle subsystem in certain bound state. For definiteness, we consider an initial state consisting of particle 1 and a bound state of (2,3) with energy $s_0$ and angular momentum $l_0$. The corresponding inhomogeneous term takes the form [see Eqs. (2.21), (2.24), and (2.26)]

$$\Phi_{l_0}^{(1)}(p,q,s)=\frac{-\frac{4}{\pi q}t_{l_0}^{(1)}(p,p_0,s-q_0^2)\delta(q^2-q_0^2)}{q_0^2-(s-s_0)}, \tag{3.17}$$

where $p_0$ and $q_0$ are the $p$ and $q$ of the initial state. Since $t_{l_0}^{(1)}$ has a pole at $s - q_0^2 = s_0$, $\Phi_{l_0}^{(1)}(p,q,s)$ can be rewritten as

$$\Phi_{l_0}^{(1)}(p,q,s) \underset{q_0^2-(s-s_0)}{=} \frac{4}{\pi q}\left[\delta(q^2-s+s_0)/\lambda_{n_0 l_0}^{(1)\prime}(s_0)(s-q_0^2-s_0)\right]\phi_{n_0 l_0}^{(1)}(p,s_0)\phi_{n_0 l_0}^{(1)}(p_0,s_0)\,, \tag{3.18}$$

where $\lambda'$ is the derivative of $\lambda$ with respect to $s$.

Now multiply both sides of Eq. (2.33) by $(s-q_0^2-s_0)/\phi_{n_0 l_0}^{(1)}(p_0,s_0)$ and then take the limit $q_0^2 \to s - s_0$. It is easily seen that all the inhomogeneous terms vanish except for $\Phi_{l_0}^{(1)}$ and that the wave function of the initial (2,3) bound state $\phi_{n_0 l_0}^{(1)}(p_0,s_0)$ is factored out of the equation. Substitution of $\Phi_{l_0}^{(1)}$ from Eq. (3.18) into Eq. (3.15) gives an explicit inhomogeneous term $\eta_{nl}^{(i)}$. Equation (3.14) can now be solved by standard numerical methods. For $s$ above the lowest branch point the kernel must be taken as the limit of $s$ approaching the real axis from above. One can either use numerical methods for complex arithematics or the Fredholm reduction given by Noyes[18] and by Kowalski.[19]

### C. Spin and Identical Particles

So far, we have not considered spin in this formulation of the Faddeev equations. For nonrelativistic atomic problems, there is no spin-orbit coupling and the effect of the spin simply appears as a multiplicative factor in the kernel[8]:

$$\mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j;s) - \mathcal{K}_{nlS,n'l'S'}^{(i,j)}(q,q_j;s,S_0) = (-1)^{S_i+S_j+S_k+S_0}[(2S+1)(2S'+1)]^{\frac{1}{2}}\begin{Bmatrix} S_j & S_k & S \\ S_i & S_0 & S' \end{Bmatrix} \times \mathcal{K}_{nl,n'l'}^{(i,j)}(q,q_j,s)\,, \tag{3.19}$$

where $S_0$ is the total spin of the three-particle system; $S$ the spin of the pair $(j,k)$; $S'$ the spin of the pair $(k,i)$; $S_i$, $S_j$, and $S_k$ the spins of the individual particles; and $\{\ \}$ denotes the $6j$ symbol. Of course, the $T$-matrix elements $\chi_{nl}^{(i)}$ should now carry an additional spin index $S$ denoting the spin of the pair $(j,k)$.

As for identical particles, the statistics require that the two-body partial wave $T$ matrix $t_l^{(i)}(p,p';E,S)$ be identically zero for certain $l$. In particular, for two spin-$\frac{1}{2}$ identical fermions, $t$ is zero for even $l$ if $S=1$ and for odd $l$ if $S=0$. As long as all the two-body $T$-matrix elements satisfy the requirement of statistics, the solution of the Faddeev equations also satisfies the statistic. The number of equations is reduced because some of the kernels become equivalent.

## IV. APPLICATION TO THE (e,H) SYSTEM

It is well-known that for the $(e,\mathrm{H})$ system, there exists only one three-particle bound state corresponding to the ground $^1S$ $H^-$ state. All the other three-particle states are unstable. They correspond to the resonant states which may be generated in the laboratory in an electron-hydrogen (atom) scattering experiment.[20,21] Theoretically it can be shown[22,23] that associated with each excited two-particle threshold (corresponding to the excited states of H atom) there exist a number of resonances supported by a potential which asymptotically goes to zero primarily as $r^{-2}$. Reasonably accurate determinations of the position and the width of a few of the lower members of the resonances have been recently carried out both theoretically[24-29] and experimentally.[21] For the bound $H^-$ state on the other hand, an accurate value for the $H^-$ detachment potential has been known for some time. A calculation of this singlet $H^-$ state and the lowest members of the resonances in both the singlet and the triplet $J=0$ series would therefore provide some insight into the feasibility of the method outlined in Sec. III.

### A. The $^1S$ $H^-$ Bound State

Since the $^1S$ $H^-$ state has a zero total angular momentum (i.e., $J=0$), Eq. (3.4) may be used for the calculation of this state. One can readily show for singlet spin multiplicity that the electron-proton interaction amplitudes for electrons 1 and 2 must satisfy the relation

$$\chi_{nl}^{(1)}(q,s) = (-)^l \chi_{nl}^{(2)}(q,s)\,, \tag{4.1}$$

and the electron-electron amplitude the relation

$$\chi_{nl}^{(3)}(q,s) = 0 \quad \text{for odd } l. \tag{4.2}$$

Equation (4.2) is simply the statement of the Pauli principle which excludes the possibility for two electrons in the singlet spin state to have odd parity. Equation (4.1) allows for the reduction of the coupled equations [Eq. (3.14)] into a pair of coupled equations. The spin factor for the kernel is unity in this case.

We write Eq. (3.14) in the matrix notation

$$\underline{\chi}(q,s) = \underline{\eta}(q,s) + \int_0^\infty dq_j^{\,2}\, \underline{\mathfrak{K}}(q,q_j;s)\underline{\chi}(q_j,s)\,, \tag{4.3}$$

with $$\underline{\chi}^\dagger(q,s) = [\chi_0^{(1)}(q,s), \chi_0^{(3)}(q,s), \chi_1^{(1)}(q,s), \chi_1^{(3)}(q,s), \chi_2^{(1)}(q,s), \chi_2^{(3)}(q,s), \ldots], \tag{4.4}$$

where each element $\chi_l^{(i)}(q,s)$ is a row with a dimension which equals the number of terms included in the off-shell two-particle amplitude $t_l^{(i)}$ [see Eq. (3.5)]. Equation (4.3) may be solved for $\chi(s)$ by digitizing the continuous variables $q$ and $q_j$ and inverting the matrix $(I - \underline{\mathfrak{K}})$

$$\underline{\chi}(s) = [I - \underline{\mathfrak{K}}(s)]^{-1}\underline{\eta}(s)\,. \tag{4.5}$$

To calculate the bound $H^-$ state, we need to determine the pole in the inverse operator $[I - \underline{\mathfrak{K}}(s)]^{-1}$. The pole may be located by locating the energy $s$ at which the determinant of the $I - \underline{\mathfrak{K}}(s)$matrix is zero.

For Coulomb interactions, the matrix elements in $\mathfrak{K}$ may be obtained analytically since both the eigenfunctions $\phi_{nl}^{(i)}$ and eigenvalues $\lambda_{nl}^{(i)}$ of the homogeneous Lippmann-Schwinger equation [Eq. (3.2)] are known explicitly [see Eqs. (3.7) and (3.8)]. It can be shown that when these explicit expressions are utilized with the help of Eq. (3.10), all the integrals needed for the evaluation of the matrix element in $\mathfrak{K}$ can be expressed in terms of the basic integrals

$$I_n(q,q_i;s) \equiv \int_{(\sqrt{2}q - q_i)^2}^{(\sqrt{2}q + q_i)^2} \frac{dp_i^{\,2}}{(p_i^{\,2} + q_i^{\,2} - s)^{n+1}}\,, \tag{4.6}$$

where we have made use of the large disparity between the electron and proton masses (i.e., $m_1/m_3 = m_2/m_3 \cong 0$). These integrals satisfy the recursion relation

$$I_{n+1} = [n/(n+1)]\{[(\xi+\zeta)^{n+1} - (\xi-\zeta)^{n+1}]/[(\xi+\zeta)^n - (\xi-\zeta)^n]\}[I_n/(\xi^2 - \zeta^2)],\quad n \geq 1\,, \tag{4.7}$$

with $$\xi = (2q^2 + 2q_i^{\,2} - s)\,,\quad \zeta = 2\sqrt{2}\,qq_i\,, \tag{4.8}$$

where the recursion relation for the $I$'s starts with

$$I_1 = 4\sqrt{2}\,qq_i/[(2q^2 + 2q_i^{\,2} - s)^2 - 8q^2q_i^{\,2}]\,. \tag{4.9}$$

As discussed before, the three-particle bound states can only occur below the branch point corresponding to the elastic threshold. In this energy region $s < -1$ Ry ($-13.605$ eV), the matrix$(I - \mathfrak{K})$ is pure real. After Eqs. (4.1) and (4.2) are utilized in Eqs. (4.3), the resultant matrix integral equations are then solved by matrix inversion [Eq. (4.5)]. By taking only the first term in the $t_l^{(i)}$ expansion [Eq. (3.5)], we found that the $H^-$ state appears at $-1.0516$ Ry below the three-particle breakup threshold. This corresponds to a detachment potential of $-0.0516$ Ry (i.e., 0.702 eV) for $H^-$ in comparison with the accurate value of $-0.0555$ Ry of Peheris.[30] The agreement is most remarkable in view of the fact that only a single $1s$ term in the $t_l^{(i)}$ expansion is used in the calculation. This then implies that all the remaining terms contribute less than 7%.

To demonstrate that all the remaining terms in the $t_l^{(i)}$ expansion contribute less than 7% is, however, a somewhat difficult task. The expansion converges in an oscillatory manner and involves large cancellations. For example, the addition of the $2s$ term pushes the $H^-$ state up very close to the elastic threshold. The $2s$ term effect is cancelled by the $3s$ term. The net result due to the inclusion of the $2s$ and $3s$ terms is to move the $H^-$ state down to $-1.061$ Ry. On the other hand, the addition of $2p$ and $3p$ terms would lower further the $H^-$ state to $-1.064$ Ry, and the addition of a $3d$ and $4s$ terms then pushes the $H^-$ state up to $-1.063$ Ry. It is clear from the numerical result that the oscillations become smaller for higher terms in the $t_l^{(i)}$ expansion. However, our results seem to converge to a value lower than the accepted value. This is probably due to systematic errors in our numerical calculations. We will return to the convergence problem in Sec. V. Perhaps it is worthwhile to note that there is a substantial continuum component in each term of the $t_l^{(i)}$ expansion because this is a Stermian function expansion, so that the symbols $1s$, $2s$, $2p$, etc. should be interpreted accordingly.

Recently, a calculation of the $H^-$ bound state has been carried out by Vesselova.[31] In this calculation the two-body interaction amplitude between the electrons $t_l^{(3)}$ was taken to be zero. As a test of our program we have considered the $t_l^{(3)} = 0$ case and obtained, as expected, an energy spectrum which is simply the superposition of two sets of hydrogenic levels.

### B. The Resonant $H^-$ States

As the total energy $s$ of the system moves above the elastic threshold, we encounter the electron-hydrogen scattering problem. The corresponding matrix $(I-\underline{\mathcal{K}})$ now becomes complex and contains branch points arising from bound states of H atom. These branch points must be treated properly in solving Eq. (4.3) for resonant states and in calculating the complex poles in $(I-\underline{\mathcal{K}})^{-1}$. As an example, we will determine the two lowest $J=0$ resonances with singlet and triplet spin states in the elastic region. We choose this example for simplicity since in the elastic energy region the branch point of concern is reduced to just the one associated with the ground hydrogen state.

For the calculation of the singlet $J=0$ resonances, one may again solve Eq. (4.3) numerically. Due to the presence of the branch points, it is difficult to maintain a desired accuracy by the standard numerical method of complex integration. However, the accuracy may be significantly improved by the Fredholm reduction method[18,19] in which the branch points are removed from the matrix to be inverted. For the present problem, the only branch point of concern is that associated with the ground H state in $\chi_0^{(1)}(q,s)$ [Eq. (4.4)]. We will now show how such a method may be adopted for the present problem.

Write for $\underline{\chi}(q,s)$ the expression

$$\underline{\chi}(q,s)=u(s)\underline{\Upsilon}(q,s) \tag{4.10}$$

where $u(s)=\chi(\sqrt{s_0},s)$ and

$$\underline{\Upsilon}^{\dagger}(s)=[\Upsilon_0^{(1)\dagger}(q,s),\ \Upsilon_0^{(3)\dagger}(q,s),\ \Upsilon_1^{(1)\dagger}(q,s),\ \Upsilon_1^{(3)\dagger}(q,s),\ \Upsilon_2^{(1)\dagger}(q,s),\ \Upsilon_2^{(3)\dagger}(q,s),\ldots], \tag{4.11}$$

where $s_0\equiv s+1$, $u(s_0)$ is a scalar function, and the $\Upsilon_l^{(i)}(q,s)$'s are columns with elements $\Upsilon_{nl}^{(i)}(q,s)$. For the purpose of calculating resonance poles, we may replace Eq. (4.3) by

$$u(s)\underline{\Upsilon}(q,s)=\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0},s)+u(s)\int_0^{\infty}dq_j^{\,2}\,\underline{\mathcal{K}}(q,q_j,s)\underline{\Upsilon}(q_j,s) \tag{4.12}$$

where we have replaced $\underline{\eta}(q,s)$[see Eq. (4.3)] by $\underline{\mathcal{K}}_{10}^{(1)}(q,s_0;s)$ since poles in $\chi(s)$ are independent of the inhomogeneous term $\eta(q,s)$[see Eq. (4.5)]. The symbol $\underline{\mathcal{K}}_{10}^{(1)}$ stands for $\underline{\mathcal{K}}_{10,nl}^{(1,i)}$ where $i$, $n$, and $l$ are the suppressed indices of $\Upsilon$. This quantity ${}_{10}^{(1)}(q,s_0;s)$ in Eq. (4.12) is chosen to make the kernel of the integral equation for $\Upsilon$ nonsingular at $q^2=s_0$. By definition of $u$, $\Upsilon_{10}^{(1)}(\sqrt{s_0},s)$ is normalized to unity. Solving Eq. (4.12) for $u(s)$ at $q^2=s_0$, we obtain

$$u(s)=\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)\Big/\Big(1-\sum_{\substack{j,n,l\\ n>l}}\int_0^{\infty}dq_j^{\,2}\,\mathcal{K}_{10,nl}^{(l,j)}(\sqrt{s_0},q_j;s)\,\Upsilon_{nl}^{(j)}(q_j,s)\Big)\,. \tag{4.13}$$

Substitution of $u(s)$ from Eq. (4.13) back into Eq. (4.12) yields

$$\underline{\Upsilon}(q,s)=\frac{\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0},s)}{\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)}+\int_0^{\infty}dq_1^{\,2}\left\{\underline{\mathcal{K}}(q,q_j;s)-\frac{\underline{\mathcal{K}}_{10}^{(1)}(q,\sqrt{s_0};s)}{\mathcal{K}_{10,10}^{(1,1)}(\sqrt{s_0},\sqrt{s_0};s)}\,\underline{\mathcal{K}}_{10}^{(1)\dagger}(\sqrt{s_0},q_j;s)\right\}\underline{\Upsilon}(q_j,s)\,. \tag{4.14}$$

Now, the kernel does not have a pole at $q_j^2=s_0$, and Eq. (4.14) contains no branch point for $s<-0.25$ Ry. It may be solved in a straightforward manner for $\Upsilon(q,s)$. Having obtained $\underline{\Upsilon}(q,s)$, $u(s)$ can be calculated by evaluating the principal part integral in Eq. (4.13), and the poles of $u(s)$ are then poles of $\chi$.

Unlike the case for the bound state, retaining only the 1$s$ term in the $t_l^{(i)}$ expansion [Eq. (3.5)] fails to give any resonance. A resonance pole is found when either the 2$s$ or the 2$p$ term is included in the $t_l^{(i)}$ expansion. This is expected since the $H^-$ resonances are closed-channel resonances[22] lying very close to the excitation threshold. The positions of the pole obtained in the 1$s$-2$s$ and 1$s$-2$p$ expansions are at $-0.286$ and $-0.291$ Ry below the three-particle breakup threshold, respectively. The position of the lowest $H^-$ resonance in the $J=0$ singlet series has been found to be at $-0.2973$ Ry both experimentally[21] and theoretically.[22–29] This seems to indicate that neither the 2$s$ nor the 2$p$ term alone is sufficiently attractive to lower the pole to $-0.2973$ Ry. From these results one may also conclude that the 2$p$ term is more attractive than the 2$s$ term.

The combined effect of the 2$s$ and 2$p$ terms, on the other hand, is much too attractive. The pole is lowered in the 1$s$-2$s$-2$p$ approximation to $-0.326$ Ry. It requires the 3$s$ term to push the pole up to $-0.3004$ Ry. The addition of the 3$p$ and 3$d$ terms move the pole further up to $-0.298$ Ry, which is closer to the value of $-0.2973$ Ry calculated in the closed-coupling approximation with correlated wave functions. Though there is a definite indication of convergence towards the value of $-0.2973$ Ry, the convergence is again oscillatory and not rapid. It is perhaps worthwhile to emphasize that the present calculation is term-by-term exact. No variational or stationary parameters were used in the calculation.

The calculated width for the lowest $J=0$ singlet resonance in the 1$s$-2$s$-2$p$-3$s$ approximation is 0.0025 Ry (0.034 eV) which is in reasonable agreement with previous calculations.[24,25,28,29] The measured width for this resonance is 0.043 eV.[21] In Fig. 4 the profile of the elastic scattering cross section in the neigh-

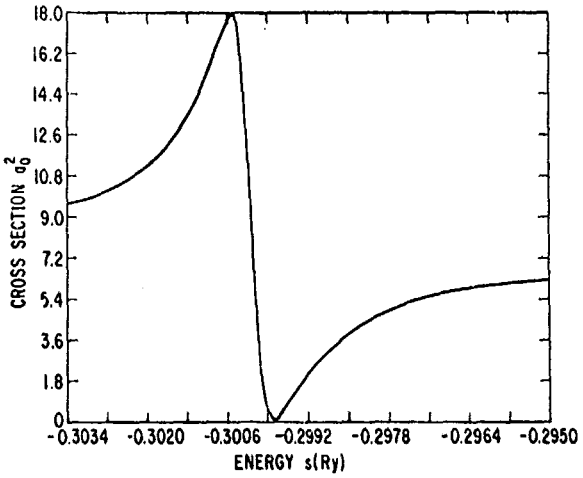


FIG. 4 Energy dependence of the singlet $J=0$ elastic scattering cross section in the neighborhood of the resonance in the $1s$-$2s$-$2p$-$3s$ approximation.

borhood of the $J=0$ singlet resonance is given. It is seen that the interference between direct and resonance scattering is important. Due to the absence of other channels, the cross section actually dips through zero at $s=-0.2997$ Ry.

For the triplet case, the electron-proton interaction amplitudes for electrons 1 and 2 must satisfy, instead of Eq. (4.1), the relation

$$\chi_{nl}^{(1)}(q,s)=(-)^{l+1}\chi_{nl}^{(2)}(q,s), \tag{4.15}$$

and the electron-electron interaction must satisfy, instead of Eq. (4.2), the relation

$$\chi_{nl}^{(3)}(q,s)=0, \quad \text{for even } l. \tag{4.16}$$

Equation (4.16) is again the statement of the Pauli principle which excludes the possibility for two electrons in the triplet spin state to have even parity. Equation (4.15) allows for the reduction of Eq. (3.14) into a different pair of coupled equations for the triplet case. The spin factor for the kernel is again unity.

The behavior of the solution for the triplet case is similar in nature to the singlet case. We obtain in the $1s$-$2s$-$2p$-$3s$-$3p$ approximation a resonance pole at $-0.257$ Ry below the three-particle breakup threshold with a width of $\sim 2\times10^{-5}$ Ry ($2.72\times10^{-4}$ eV) which are in reasonable agreement with the previously calculated values.[25,29]

## V. CONCLUDING REMARKS

The method presented in Sec. III provides a practical way of solving the Faddeev equation for Coulomb potentials below three-particle breakup threshold. It is seen, from the example in Sec. IV, that by retaining only a few leading terms in the series a reasonably accurate value is obtained. The interesting problem is then to investigate the convergence of the remaining terms in the series. This is, however, a somewhat difficult task, since, as was pointed out in Sec. IV, the expansion converges in an oscillatory manner and involves large cancellations. The net sum of all the terms, considered as a whole, constitutes, nevertheless, a small correction. It is then feasible that a perturbation scheme in which the sum of the contribution of the remaining terms is treated as a perturbation may be developed. In this concluding section, we outline such a perturbative scheme.

Let us consider the problem of determining the poles in the inverse operator in Eq. (4.5) by examining the energy dependence of the determinant Det $\{I-\underline{\mathcal{K}}(s)\}$. We can partition the matrix as

$$I-\underline{\mathcal{K}}(s)=\underline{B}+\underline{\mathcal{E}}=\underline{B}\{I+\underline{B}^{-1}\underline{\mathcal{E}}\}, \tag{5.1}$$

where $\underline{B}$ is a square matrix consisting of elements obtained in a truncated expansion including the leading terms in the series and $\mathcal{E}$ is the remainder. Utilizing the relation between the determinant and the trace of the logarithm of the corresponding matrix,

$$\mathrm{Det}\underline{A}=\exp\{\mathrm{Tr}(\ln\underline{A})\}, \tag{5.2}$$

we have

$$\mathrm{Det}\{I-\underline{\mathcal{K}}(s)\}=\mathrm{Det}\underline{B}\exp\{\mathrm{Tr}[\ln(1+\underline{B}^{-1}\underline{\mathcal{E}})]\}=\mathrm{Det}\underline{B}\{1+\mathrm{Tr}\underline{B}^{-1}\underline{\mathcal{E}}-\tfrac{1}{2}\mathrm{Tr}(\underline{B}^{-1}\underline{\mathcal{E}}\underline{B}^{-1}\underline{\mathcal{E}})+\cdots\}. \tag{5.3}$$

Defining $\underline{C} = \underline{B}^{-1}$, we have

$$\mathrm{Det}\{I - \underline{\mathcal{K}}(s)\} = \mathrm{Det}\underline{B}\Big[1 + \sum_{\alpha=m+1}^{n} \epsilon_{\alpha\alpha} - \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m}\sum_{\gamma=m+1}^{n} c_{\alpha\beta}\epsilon_{\beta\gamma}\epsilon_{\gamma\alpha} - \tfrac{1}{2}\sum_{\alpha=m+1}^{n}\sum_{\lambda=m+1}^{n} \epsilon_{\lambda\alpha}\epsilon_{\alpha\lambda} + \tfrac{1}{2}\Big(\sum_{\alpha=m+1}^{n} \epsilon_{\alpha\alpha}\Big)^2 + \cdots\Big], \tag{5.4}$$

where $\epsilon_{ij}$ and $c_{ij}$ are the elements of matrices $\underline{\mathcal{E}}$ and $\underline{C}$ respectively, $n$ is the order of the matrix while $m$ is the order of the submatrix corresponding to the truncated expansion. This then provides a systematic way of investigating the convergence problem.

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# H(2$p$) EXCITATION RESONANCES IN ($e$-H) SYSTEM NEAR THRESHOLD*

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High-resolution electron-impact measurements reveal that just above the threshold for excitation of the 2$p$ level of atomic hydrogen there is a complicated resonance structure, part of which had not previously been predicted or observed.

In this note we discuss our recent measurements of the resonance structure found in the total cross section for the production of Lyman-$\alpha$ from the reaction

$$e + \mathrm{H}(1s) = e + \mathrm{H}(2p) \longrightarrow \mathrm{H}(1s) + \text{Lyman-}\alpha.$$

The observed structure is associated with the temporary formation of one or more $H^-$ compound states in the $(2s)^2$, $(2p)^2$, or $(2s, 2p)$ doubly excited configurations. These "potential" resonances are of the same configurations as the resonances previously studied in the elastic channel below the first inelastic threshold.[1]

It has previously been observed, both theoretically[2-4] and experimentally,[5] that the excitation cross section does not follow what is normally considered Wigner's law. The most recent calcualtions have demonstrated that near threshold there is at least one resonance. However, a major point of this report will be to show that the resonance structure in the threshold region is more complicated than has been suggested thus far by theory. In the paper which follows, a partial explanation of this observation is given by Marriott and Rotenberg.[6] In a subsequent experimental paper, the details of our experimental technique, our total cross-section measurements, and our measurements of the resonances below and above the $n=3$ level will be discussed.

A modulated rectangular beam of H atoms (more than 85% pure) is crossed with a rectangular beam of electrons with an energy distribution (the width of the Gaussian energy distribution at half-maximum) of 0.07 eV. Electrons from a 127° electron-energy selector enter a magnetic- and electric-field free region, cross the modulated H-atom beam from below, and then pass into a collector in which a crossed electric field can be applied to collect all the electrons in the beam. When this field is removed the electrons pass through the collector region into a second, rotatable, electrostatic energy analyzer which measures the energy and angular distribution of the electrons. Photons from the interaction of the electron and hydrogen atoms are detected at an angle of 54.5° with respect to the direction of the electrons. At this angle the observed signal

is proportional to the total $2p$-excitation cross section.[7]

Ions from the interaction region are accelerated along the atomic-beam axis into a Paul mass filter. As in previous experiments[1,6] the linear extrapolation of the ionization efficiency curve to its energy axis is used as a calibration reference point for the electron energy scale. As has already been shown, this point is approximately 0.03 eV above the real ionization threshold.[8]

For each experimental run, data were collected automatically over a period which often exceeded 100 h. The instrument was programmed to step through a prescribed energy interval which in this experiment is usually 0.90 eV taken in 0.015-eV steps. The residence time for each energy step was normally 60 sec. The data were collected digitally, i.e., for each energy interval, the signal plus background, the background, and the electron current were recorded on punched tape to be processed later by the computer. Every 12 to 15 h the process was interrupted and an ionization efficiency curve for the collision

$$H(1s) + e = H^+ + 2e$$

was taken to make sure that the electron energy scale for excitation remained constant. Through all of our experiments the ionization reference point remained constant to within ±0.015 eV.

Because particular attention was to be focused upon the details of the structure which appeared in our excitation curves, it was necessary to make certain that none of the structure observed was due to radiation from the collisions of the electrons with $H_2$ molecules residual in our H-atom beam or with $H_2$ which formed part of the background gas. It has already been recognized[7] that the oxygen gas filter which is normally placed in front of the Lyman-$\alpha$ detector, although transparent to Lyman-$\alpha$, also passes some molecular radiation. However, it has now been verified by our experiments that the electron energy threshold for production of this molecular radiation is in the vicinity of 11.3 eV, well above the range of interest for this report. Consequently, such radiation cannot have affected our results.

In Fig. 1(a), we give a comparison of our data with the earlier low-resolution experimental results of Chamberlain, Smith, and Heddle[5] and with two calculations on this system, both by Taylor and Burke.[4] In Fig. 1(b), the results of Taylor and Burke are shown as modified by folding into their correlation calculation our experimental electron energy distribution. The experimental data reported here have been normalized to the Born approximation at high energies by a procedure to be discussed in detail in a later paper.[9] The results of Chamberlain, Smith, and Heddle are also normalized to theory near threshold in the manner given by Burke, Taylor, and Ormonde.[4]

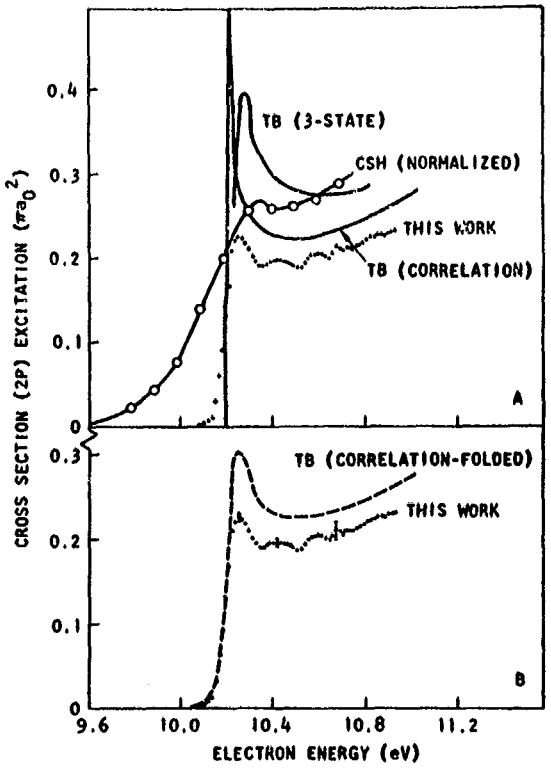


FIG. 1. (a) Our data for the excitation of H($2p$) (this work), together with earlier measurements by Chamberlain, Smith, and Heddle (CSH) of the Lyman-$\alpha$ excitation cross section (for radiation observed at 90° to the direction of the bombarding electrons). Also shown are two theoretical calculations: the three-stage close-coupling calculations of Taylor and Burke [TB (3 state)] and the three-state-plus-correlation calculation of Taylor and Burke [TB (correlation)]. (b) Comparison of our data with the calculated cross section of Taylor and Burke into which has been folded our experimental energy distribution 0.07 eV.

The sharp rise in the excitation cross section at threshold has been predicted by Damburg and Gailitis[3] from a close-coupling approximation calculation which includes the lowest three states of the H atom, i.e., the $1s$, $2s$, and $2p$ states. Subsequent three-state close-coupling calculations by Taylor and Burke,[3] shown as TB (3-state) in Fig. 1(a), have used a finer energy grid to show that within 0.03 eV of the threshold, there is a sharp resonance in the $^1P$ channel of

the temporary $H^-$ doubly excited compound state. A modified calculation, in which the interaction potential contains an additional term to describe the electron-electron interaction (correlation), shown as TB (correlation) in Fig. 1(a), lowers the total cross-section value, shifts the position of the resonance closer to threshold, and considerably reduces its width.

The results of Chamberlain, Smith, and Heddle using an electron beam with a resolution of 0.35 eV, and observing Lyman-$\alpha$ emitted at 90° to the direction of the electron beam, show that the cross section near threshold is finite as predicted. By assuming various shapes for the excitation cross section into which they folded their known electron-energy distribution, they were able to suggest that the cross section near threshold contained a peak. Subsequently, Burke, Taylor, and Ormonde[4] theoretically identified this peak and showed that their calculations were consistent with the measurements. With our measurements, which have been made with an electron-energy resolution of 0.07 eV, the predicted sharp onset at threshold and the $^1P$ potential resonance near threshold are clearly defined. Now, however, our data reveal the presence of second and third maxima which have not previously been reported. This second maximum is statistically real, its height being approximately twice the rms error, while the third maximum is not yet statistically sound although its presence has been observed in all our data.

In Fig. 1(b) we show our data in comparison with the three-state close-coupling-plus-correlation calculation of Taylor and Burke[3] into which we have folded our electron energy distribution. The agreement at threshold and over the first peak is good, thus giving credence to the calculated position of the resonance at 10.214 eV; however, the discrepancy in widths is large enough so that we suggest that the width of their resonance should be slightly in excess of the suggested 0.015 eV.[10]

What is the second peak which appears in our data? One possible explanation is that there is more than one potential resonance in the $^1P$ channel. Another possible explanation, which is discussed in the following paper by Marriott and Rotenberg,[6] is that the second peak is part of the first resonance and is not really a separate resonance at all.

One possible explanation for the conjectured third peak is that it, too, is part of a series of potential resonances. Another, and perhaps a more reasonable explanation, is that this is structure which appears in some channel other than the $^1P$.

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