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Absolute cross sections for excitation of neon by impact of 20-180 keV H, H₂ and He ions

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ABSOLUTE CROSS SECTIONS FOR EXCITATION
OF NEON BY IMPACT OF 20-180 keV
H, H₂ AND HE IONS

by

GEORGE WILLIAM YORK, JR., 1945-

A DISSERTATION

Presented to the Faculty of the Graduate School of the

UNIVERSITY OF MISSOURI - ROLLA

In Partial Fulfillment of the Requirements for the Degree

DOCTOR OF PHILOSOPHY

in

PHYSICS

1971

T2620
94 pages
C.1
PUBLICATION THESIS OPTION

This thesis has been prepared in the style utilized by the Physical Review. Pages 1-52 will be submitted for publication in that journal. Appendix A has been accepted, in part, for publication in the Review of Scientific Instruments. Appendix B has been added for purposes normal to thesis writing.
ABSTRACT

The technique of heavy-ion energy-loss spectrometry has been used to measure excitation cross sections for the \((2p^5)3s\) and \((2p^5)3p\) electronic configurations of Neon. The incident particles used were \(H^+\), \(H_2^+\) and \(He^+\) at impact energies from 20-180 keV. The results are compared with previous optical measurements of the emission cross sections of lines from these levels as excited by \(H^+\) and \(He^+\) impact. Agreement is not good, either in shape or in absolute magnitude for excitation of the \((2p^5)3s\) configuration. However, agreement is surprisingly good for excitation of the \((2p^5)3p\) configuration. A curve fitting technique has been applied to extract relative singlet-triplet cross sections for levels within the \((2p^5)3s\) configuration. Almost no triplet excitation is observed for \(H^+\) and \(H_2^+\) impact. The former is expected while the latter is somewhat surprising. Significant triplet excitation is observed only for \(He^+\) impact.
ACKNOWLEDGEMENTS

The successful completion of this project was the result of the untiring efforts of many persons who contributed indispensable technical and moral support. Foremost, of course, is my advisor, Dr. John T. Park. I acknowledge with deep gratitude his diligent efforts and indomitable spirit, which encouraged me to continue to the completion of the project.

Thanks are also due to Dr. David H. Crandall who, in Dr. Park's absence, not only supplied technical assistance, but was that most valuable of assets - a very good friend.

Appreciation is also due to Victor Pol for his efforts in taking the data and maintaining the apparatus, many times in obvious sacrifice of his own progress.

I would also like to thank the members of both the technical staff and the Faculty of the Physics Department for their many contributions.

Last, but by no stretch of the imagination least, I owe my deepest appreciation to my wife, Susan, for her many sacrifices and for her unfailing belief in me. I hope that I may prove that her belief was not misplaced.
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I. INTRODUCTION

There has been considerable recent interest in the properties of Neon as embodied in collision cross sections. Investigations have been conducted by bombarding Neon with low energy ions\textsuperscript{1-3} and with electrons at energies ranging from threshold to several hundreds of eV.\textsuperscript{4,5}

The extensive work of Coffey et al\textsuperscript{3} on inelastic and elastic scattering of He\textsuperscript{+} by Ne at energies below 500 eV has indicated the wealth of information obtainable by collision spectroscopy. In this low energy range, the observed patterns in the data can be explained quite reasonably in terms of molecular curve crossings which, in turn, yield valuable information concerning the nature of interatomic forces. However, at energies in the keV range, the simple curve crossings do not explain the observed phenomena and hence probably do not provide the dominant mechanism for inelastic processes in this energy range.

To date, very little emphasis has been placed on
the acquisition of data which would help in our understanding of these processes. Among the few reported experimental efforts in this area are the works of DeHeer et al,\textsuperscript{6,7} van Eck et al\textsuperscript{8} and Jaecks et al,\textsuperscript{9} who have measured emission cross sections for spectral lines of Neon induced by proton and He\textsuperscript{+} impact at energies up to 35 keV. Thomas and Gilbody\textsuperscript{10} have bombarded the noble gases with high energy (100-400 keV) Helium ions but were not able to observe emission corresponding to excitation of atomic Neon lines.

We have attempted to fill this gap in our knowledge by measuring cross sections for excitation of the two lowest electronic configurations of Neon by impact of H, H\textsubscript{2} and He ions using the technique of heavy-ion energy-loss spectrometry\textsuperscript{11}. The results presented cover the energy range 20-180 keV and are, to the authors' knowledge, the first measurements of the absolute cross sections for excitation of Neon in this energy range.

The properties of Neon are of interest because of the use of Neon in lasers, as a possible charge transfer agent for neutral injection into controlled thermonuclear plasmas,\textsuperscript{12} and because of its deviation from Russell-Saunders (LS) coupling.\textsuperscript{13}
II. EXPERIMENTAL

The apparatus and philosophy of heavy-ion energy-loss spectrometry has been discussed in detail elsewhere. The following is a brief description of the apparatus, together with a more complete description of the angular acceptance of the apparatus. The latter is required since Neon is more massive than previous targets.

Ions produced in a Colutron low-voltage discharge source are accelerated and steered into a target chamber containing the gas under study. After traversing the scattering chamber, the forward scattered beam is magnetically momentum analyzed to obtain the particular ion species of interest. This beam is then decelerated to a low, well-defined energy and energy analyzed by a $127^\circ$ electrostatic analyzer. Detection is accomplished by an 18 stage EMI electron multiplier. Target density is monitored by an MKS Baratron, which is taken as the laboratory standard.

Spectra differential in energy loss are obtained by slowly increasing the potential difference between the accelerator and decelerator terminals. Whenever the increased potential difference compensates for a discrete energy loss of the projectile-target system, a peak is detected in the spectrum. It should be noted that the technique of compensating for the energy lost in the
collision ensures that all detected particles have traversed similar trajectories through the mass and energy analyses and the deceleration column. Thus, cross sections obtained with this device are absolute to the extent that they are independent of detection efficiency.

Recent modifications have been made which have permitted determination of the energy loss scale to an accuracy of ±0.03 eV. This is accomplished by utilizing a high precision voltage calibrator to establish the potential difference between the terminals and hence the energy loss scale. The fact that the energy loss scale is not known to the accuracy of the power supply, as one would expect, is due to varying contact potentials within the ion source which introduce small shifts in the initial energy of the beam.

The design of the apparatus is such that only the extreme forward scattered particles are detected. The maximum scattering angle is determined by the geometry of the scattering chamber. For this study, two scattering chambers were used. One consists of a chamber 6.31 cm long defined by 0.051 cm-diam orifices. This chamber is the same as that used in all previous publications. The second chamber has recently been completed for use in studies of doubly differential (angle and energy loss) scattering cross sections. It consists of a chamber 1.0
cm long defined by 0.025 x 0.025 cm orifices. The incident angle of the beam is defined by the entrance aperture of the scattering chamber and an identical aperture located at the end of a tube 20.3 cm in length. Similarly, the exit angle is defined by the exit aperture of the scattering chamber and another 0.025 x 0.025 cm aperture located at the end of a tube 25.4 cm long.

If we assume a parallel beam incident upon the scattering chamber, the maximum scattering angle is 8.1 x 10^{-3} rad in the case of the first scattering chamber, and 1.3 x 10^{-3} rad for the second. The true maximum scattering angle is, of course, modified by the acceptance angle subtended at the scattering center by the detection apparatus. Geometrically, the angle is defined by the analyzer entrance slit located at the exit of the deceleration column. This slit is horizontal with a vertical width of 0.005 cm. This yields a maximum exit scattering angle of 1.6 x 10^{-5} rad, which is much smaller than that defined by either of the scattering chambers. However, the geometric acceptance angle of the analyzer represents an absolute lower limit on the angle of scatter. In actual practice, the ion optics of the decelerator column tend to focus the scattered beam onto the analyzer slit. Experimentally, it has been shown that this focusing results in a compression of the beam by a fac-
tor of about 5 over that predicted by the assumption of straight line trajectories. If we use this experimental relation, we calculate the minimum acceptance angle of the detector to be approximately $2 \times 10^{-4}$ rad. The actual scattering angle may be somewhat larger due to the presence of non-parallel components in the beam. Experiment has shown that, with no gas in the scattering chamber, the transmitted intensity is one-half the peak value at an angle of $\pm 5 \times 10^{-4}$ rad. Thus, although scattering angles as large as $10^{-3}$ rad are conceivable, a better estimate of the average acceptance angle, including the initial angular divergence of the beam is about $\pm 5 \times 10^{-4}$ rad.

Previous experimental results have shown that heavy particle scattering is confined predominately to the forward direction in the energy range of the present experiment. However, in the case of Neon, the results of Coffey et al. have indicated that, at low velocities of approach, angular scattering becomes appreciable, to the extent that there is almost no forward scattering. Since the velocity at which the dominant excitation mechanism ceases to be due to molecular curve crossings is not well known, the cross sections reported here should not be considered, in the lower velocity limit, total excitation cross sections. Rather, they should be
viewed as cross sections for inelastic scattering in the forward direction integrated over an acceptance angle of $5 \times 10^{-4}$ rad in the polar angle and over an acceptance angle of $1.3 \times 10^{-3}$ rad in the azimuthal angle. At impact energies above 50 keV for protons, the data of Barat and Houver$^{23}$ indicate that the results may be considered to be essentially equivalent to the doubly differential cross section integrated over all angles.

The mathematical details by which cross sections may be extracted from the data have been discussed in detail by Schoonover.$^{20,24}$ Basically, the analysis may be expressed in terms of differential equations relating the loss and gain terms of various partial beams. For our case, the equation for the incident, monoenergetic, zero-energy-loss component of the beam can be written

$$dI_{10} = -I_{10}(\sigma_c + \sigma_j + \sigma_e)dx$$  \hspace{1cm} (1)$$

where $I_{10}$ represents the monoenergetic beam, $\sigma_c$ is the cross section for electron capture, $\sigma_j$ is the total inelastic scattering cross section, $\sigma_e$ is the cross section for elastic scattering beyond the acceptance angles of the apparatus and $n$ is the target particle density, $dx$ being a differential element of path length. Similarly, the equation representing the particles which have under-
gone a specific energy loss transition resulting in an excitation of the target particle can be written

\[ \frac{dI_{1a}}{dx} = I_{10} \sigma_a \text{nd}x - I_{1a}(\sigma_c + \sigma_j + \sigma_e) \text{nd}x \]  

(2)

where \( I_{1a} \) represents the current due to the transition having the cross section \( \sigma_a \) for excitation with scattering within the acceptance angle. The loss terms are as defined previously, ignoring the small energy difference for those particles which have undergone the transition.

Exact solution of these equations subject to the boundary conditions \( I_{10} = (I_{10})_i \) and \( I_{1a} = 0 \) at \( x = 0 \) yields the detectable current due to the transition, \( (I_{1a})_f \), in terms of the detected zero-energy-loss component, \( (I_{10})_f \). That is,

\[ (I_{1a})_f = n \ell \sigma_a (I_{10})_f \]  

(3)

where \( \ell \) is the effective scattering length. Since the apparatus has a finite energy resolution, the actual detected current is a convolution of the dispersive effects of the apparatus with the initial energy spread of the beam and the effects of the target gas. That is, the detected energy loss spectrum, \( R(\xi) \), as a function of the energy loss, \( \xi \), can be written as
\[ R(\xi) = n\lambda \int \phi(\xi - \xi') \frac{d\sigma}{d\xi} d\xi' \]  

(4)

where \( \phi(\xi) \) is a convolution of the dispersive effects of the apparatus with the initial energy spread of the beam, and \( d\sigma/d\xi \) is the doubly differential cross section integrated over the instrument acceptance angles. \( n \) and \( \lambda \) are as defined previously. Then the experimental equation for determination of \( \sigma_a \) becomes

\[
\sigma_a = \frac{1}{n\lambda} \left\{ \frac{\int_{\Delta\xi_a} \int \xi R(\xi) d\xi}{\int_{\Delta\xi_o} \phi(\xi) d\xi} - \frac{\int_{\Delta\xi_o} \phi(\xi) d\xi}{\int_{\Delta\xi_o} \phi(\xi) d\xi} \right\} 
\]

(5)

The integration limits, \( \Delta\xi_a \) and \( \Delta\xi_o \), are the energy loss intervals over which the spectrum is non-zero for the transition and monoenergetic beams, respectively. Application of this equation implicitly assumes that the spectrum drops essentially to zero on both sides of the transition peak. That is, the energy loss associated with the transition must be sufficiently remote from neighboring processes that the finite resolution of the apparatus does not introduce contributions from these nearby processes to the peak under evaluation.

All data were obtained in the form of energy loss-current data pairs punched on paper tape. The required integrals were then obtained numerically by application
of Simpson's rule using a small digital computer. All data were obtained at target thicknesses for which 
\((I_{1a})_f/(I_{10})_f\) was a linear function of target particle density, that is, under single collision conditions.
III. ENERGY LOSS SPECTRA

Typical energy loss spectra obtained for heavy ion impact on Neon are shown in Fig. 1 for the three ionic projectiles used in this study. The data shown are unretouched computer plots of the apparent differential cross section as a function of energy loss. The term apparent here means that the instrumental resolution function has not yet been unfolded from the experimental results. However, all other experimental parameters have been removed in accordance with the differential form of Eq. 3 of Sec. II.

Absolute cross sections for excitation of an electronic configuration of Neon are obtained by simple numerical integration over the observed peaks in the spectra. The three peaks observed correspond, in order of increasing energy loss, to the \((2p^5)3s,3p\) and \(4s\) configurations of Neon.

The level structure within these configurations is shown in Fig. 2. The data presented is taken from the tables of Moore\(^2\text{5}\). The energy level structure is shown to scale on the extreme left. The energy scales are then expanded for the \((2p^5)3s\) and \((2p^5)3p\) configurations in order to show the detail. The appropriate LS and jj term values are listed for each level in the center of the figure. Various important optically allowed tran-
FIGURE 1

TYPICAL APPARENT DIFFERENTIAL ENERGY LOSS CROSS SECTIONS. The data shown are unretouched computer plots for each of the three ions used in this study. The impact velocity in all cases is $2.76 \times 10^8$ cm/sec.
Figure 1

- $H^+\rightarrow\text{Ne}$
- $H_{2}^{+}\rightarrow\text{Ne}$
- $\text{He}^{+}\rightarrow\text{Ne}$

$\frac{d\sigma}{d\xi}$ (10^{-18}\text{cm}^2/\text{ev}-\text{atom})

ENERGY LOSS, $\xi$, (eV)
FIGURE 2
ENERGY LEVEL DIAGRAM OF NEON. The data is taken from Moore (Ref. 25). The structure is shown to scale on the extreme left. The scale is then expanded to the right to show the detail of the $({2p}^5)3s$ and $({2p}^5)3p$ configurations. Appropriate LS and jj term designations are listed in the center, and important optically allowed transitions under assumptions of LS coupling are shown on the left, while those allowed under assumptions of jj coupling are shown on the right. All transition wavelengths are given in units of Angstroms.
Figure 2
sitions are shown. Those allowed under assumptions of LS coupling are shown on the left column, while those allowed under assumptions of jj coupling are shown on the right column.

The formalism which has been developed for describing the coupling in two electron spectra can be carried over to Neon (and the other rare gases) if we use the angular momenta of the unfilled p shell in place of that of the inner electron. This formalism has been described in detail by Cowan and Andrew.\textsuperscript{26} For the lower excited states of Neon, LS coupling is assumed to be valid. In their notation, the coupling can be written as

\[ [(\vec{l}_C, \vec{s}_2) \vec{L}, (\vec{s}_C, \vec{s}_2) \vec{S}] \vec{J} \] \hspace{1cm} (6)

where \( \vec{l}_C, \vec{s}_2 \) and \( \vec{s}_C, \vec{s}_2 \) are the orbital and spin angular momenta of the unfilled p core and the excited electron, respectively. This expresses the fact that the Coulomb interaction is larger than the spin-orbit interaction and thus the total orbital angular momentum \( \vec{L} = \vec{l}_C + \vec{l}_2 \) and spin angular momentum \( \vec{S} = \vec{s}_C + \vec{s}_2 \) are good quantum numbers.

As the outer electron is promoted to higher excited states, the levels are observed to occur in pairs. This intermediate pair structure leads to a description of the coupling intermediate between pure LS and pure jj
which is called \( jK \) coupling and can be expressed as

\[
\left[ (\hat{\mathbf{L}}_c, \hat{\mathbf{S}}_c) \hat{\mathbf{j}}_c, \hat{\mathbf{L}}_2, \hat{\mathbf{S}}_2 \right] \hat{\mathbf{J}}
\]

(7)

Now the spin-orbit coupling of the core becomes the dominant interaction, with the electrostatic interaction becoming the second most important one. In this case, then, the total orbital angular momentum and spin angular momentum are no longer good quantum numbers. In all cases, however, the total angular momentum, \( \hat{\mathbf{J}} \), is a good quantum number and the actual wavefunctions for any state of intermediate coupling can be expressed in terms of a linear combination of basis functions for any of the pure coupling cases. Thus, the wavefunctions for the 3s level can be written as combinations of the LS basis functions:

\[
\begin{align*}
\psi(1s_2) &= \hat{\alpha} \phi(1P_1) + \hat{\beta} \phi(3P_1) \\
\psi(1s_3) &= \phi(3P_0) \\
\psi(1s_4) &= -\hat{\alpha} \phi(1P_1) + \hat{\beta} \phi(3P_1) \\
\psi(1s_5) &= \phi(3P_2)
\end{align*}
\]

(8)

where the notation on the left is the Paschen notation with the subscript increasing with decreasing energy. We note that mixing only occurs for levels with the same value of \( J \) and that the 1s\(_3\) and 1s\(_5\) levels remain pure triplets. For Neon, the coefficients are \( \hat{\alpha}=0.964 \),
\( \beta = 0.266 \) \(^{27}\) yielding an LS purity of 93\% for the \((2p^5)3s\) configuration.

A test of the coupling is provided by heavy particle impact. For proton impact, transitions involving a change in multiplicity are expected to be forbidden since this would constitute a violation of the Wigner spin conservation rule\(^{28}\). Essentially, this rule states that the total spin of the colliding system must be conserved in the collision. The rule is expected to be rigorous when the spin-orbit interaction is small. That is, under conditions of good LS coupling. The rule has been experimentally verified for proton impact upon Helium\(^{29-31}\).

When the spin-orbit interaction becomes large, however, the total spin no longer remains a good quantum number. In this case, the Wigner spin rule loses rigor and proton impact excitation of "triplet" states is allowed. For impact by electrons or heavy particles which carry an electron, excitation can take place by electron exchange, regardless of the type of coupling.

While the separations of the levels within the \((2p^5)3s\) configuration are much too small to be resolved by the energy loss spectrometer, an appreciable contribution due to excitation of the triplet levels should produce a detectable shift in the energy-loss location of the peak corresponding to the 3s configuration.
We have made a systematic study of the energy loss associated with the 3s peak as a function of ion type and impact energy. The results indicate that for protons, the energy loss location is 16.83 eV over the entire range of impact energies. For $\text{H}_2^+$ impact, the location at 30 keV is 16.74 eV but rapidly increases to 16.83 eV at 60 keV. The energy loss is then constant over the remainder of the energy range. For Helium ions, however, the energy loss is 16.74 eV at 20 keV and very slowly increases to 16.83 at 170 keV. The energy shift is very nearly monotonically increasing with increasing impact energy.

These data imply that, at least for the 3s level, LS coupling provides a reasonable description of the Neon atom, in agreement with the results obtained theoretically by Fajen.\textsuperscript{5,27}

A curve fitting technique has been developed to express in a more quantitative manner the results described above. The information obtained by this method is described in Sec. V.

The data resulting from direct integration over the peaks corresponding to the two lowest electronic configurations is presented in the next section. Data are presented only for the $\text{(2p}^5\text{)}3s$ and 3p configurations because the energy resolution was not sufficient to resolve the $\text{(2p}^5\text{)}4s$ peak from the ionization continuum.
IV. DATA

In this section, data are presented for excitation of the sum of levels in the \((2p^5)3\text{s}\) and \((2p^5)3\text{p}\) electronic configurations of Neon. The error bars in all cases represent a vectorial (r.m.s.) addition of one standard deviation and of an estimated 10% systematic error, largely due to uncertainties in the pressure measurements. Each datum point represents approximately 20 data trials.

A. 3s Level

The results obtained for proton impact excitation of the 3s level are shown in Fig. 3. These results were obtained using the second scattering chamber discussed in Sec. II since the angular spread of the incident beam is smaller for this chamber as compared to the original scattering chamber. However, the results agree, within experimental error, with a previous set of preliminary data taken with the original scattering chamber\(^{32}\). The curve shown has the general shape of an optically allowed transition even though it has not yet begun to decrease at our highest energy (160 keV). It appears to have leveled off with a maximum value of \(\sim 8 \times 10^{-18} \text{ cm}^2\).

There are no previous experimental results for excitation of this level with which to compare our results. The sole previous work for proton impact in this energy
FIGURE 3

ABSOLUTE CROSS SECTION FOR EXCITATION OF THE \( (2p^5)3s \) CONFIGURATION OF NEON BY H\(^+\) IMPACT. The open circles are present data. The closed circles are the emission cross section data of DeHeer et al (Ref. 6).
Figure 3
range is that of De Heer et al\textsuperscript{6,7}, van Eck et al\textsuperscript{8} and Jaecks et al\textsuperscript{9}. They have not measured excitation cross sections directly, but have measured emission cross sections by detection of the radiation from the subsequent decay of the excited Neon target. Such cross sections can be converted to excitation cross sections provided one knows the appropriate transition probabilities and emission cross sections for higher lying states. For Neon, the recent work of Bridges and Wiese\textsuperscript{33} has provided accurate transition probabilities for the 3p levels of Neon. However, all of the necessary emission cross sections have not been measured and no attempt was made, therefore, to convert the emission data to excitation cross sections. To provide a comparison, however, the emission data is also shown in Fig. 3.

Agreement is not good, either in shape or in absolute magnitude. The discrepancy in magnitude is not surprising, both in view of the differences in measured quantities and in view of the inherent difficulties of the optical method for this level. Emission from the 3s level lies in the vacuum ultraviolet where standard sources are not available for calibration purposes.

The difference in shape is somewhat surprising, however. The decrease of our data at lower energies compared to the emission results could be due to increased enhancement,
at low impact velocities, of scattering to angles greater than our acceptance angle. There is no explanation at present, though, for the region in which our data are higher. All systematic errors associated with the present method, such as loss due to scattering, would tend to make our cross sections too low. In addition, the crossover cannot be attributed to the differences in measured quantities since, for this level, the only difference between emission and excitation cross sections can be cascade contributions from higher levels, which would tend to make the emission data higher than the excitation data.

The data for excitation by H$_2^+$ and He$^+$ are shown in Figs. 4 and 5, respectively. Both ions show the same behavior with impact velocity as that observed for protons. In both cases, the onset is slightly less rapid than for protons and the maximum value obtained by He$^+$ is slightly smaller. There are no other data available for comparison with our H$_2^+$ data. The small increase in the cross section at 20 keV appears to be real. Experimental difficulties prevented extension of the data to lower energies to see if another process is becoming dominant. It should be noted here that the cross sections reported here for H$_2^+$ are for excitation without simultaneous dissociation of the projectile. Excitations which occur with dissociation are not observable with the present apparatus.
FIGURE 4

ABSOLUTE CROSS SECTION FOR EXCITATION OF THE (2p$^5$)3s CONFIGURATION OF NEON BY H$_2^+$ IMPACT.
Figure 4
FIGURE 5

ABSOLUTE CROSS SECTION FOR EXCITATION OF THE
\((2p^5)3s\) CONFIGURATION OF NEON BY He\(^+\) IMPACT.
The open circles are present data. The closed circles are the emission cross section data
of DeHeer et al (Ref. 6).
Figure 5
The emission cross section data of DeHeer et al.\textsuperscript{6,7} and van Eck et al.\textsuperscript{8} are shown for comparison with our He\textsuperscript{+} data in Fig. 5. The discrepancy in shape noted in the case of proton impact is also apparent, to a much greater degree, for the case of He\textsuperscript{+} impact. The increase in cross section with decreasing impact energy for this system has also been observed by Coffey et al.\textsuperscript{3} and Liples et al.\textsuperscript{1} for very low impact energies (<1 keV). It is possible that the formation of quasi-molecular states is becoming important at the lower velocities of our experiment, with resultant scattering at large angles.

B. 3p Level

The results obtained for ionic impact excitation of the \((2p)\textsuperscript{5}3p\) electronic configuration of Neon are shown in Figs. 6, 7 and 8 for H\textsuperscript{+}, H\textsubscript{2}\textsuperscript{+} and He\textsuperscript{+} impact, respectively. All levels of this configuration are optically forbidden from the ground state by parity selection rules. (\(\Delta\ell\) of the excited electron is zero)

All of the data exhibit nearly identical behavior. In all cases, the slope of the onset, as a function of impact velocity, is very nearly identical, within the experimental error. In addition, the cross section in each case reaches a maximum value of \(\approx 4.5 \times 10^{-18} \text{ cm}^{2}\) at an impact velocity of \(\approx 3 \times 10^{8} \text{ cm/sec}\). According to the adiabatic criterion of Massey\textsuperscript{33}, this would correspond to an interaction distance on the order of 7 \(\ell\), which is
FIGURE 6

ABSOLUTE CROSS SECTION FOR EXCITATION OF THE
(2p^5)3p CONFIGURATION ON NEON BY PROTON IMPACT.
The open circles are present data. The closed
circles are the emission cross section data of
DeHeer et al, van Eck et al and Jaecks et al
(Refs. 6,8 and 9). Our data for excitation of
this level by H_2^+ and He^+ impact are also shown
to illustrate the similarity in the onset of
the cross section function for the three ions.
The boxes are the H_2^+ data, while the triangles
are the He^+ data. The latter data is plotted
as a function of velocity (upper scale) only.
Figure 6
FIGURE 7

ABSORLUTE CROSS SECTION FOR EXCITATION OF THE
(2p^5)3p CONFIGURATION OF NEON BY H^+ IMPACT.
Figure 7

VELOCITY ($10^8$ cm/sec)

CROSS SECTION ($10^{-18}$ cm$^2$)

IMPACT ENERGY (keV)
FIGURE 8

ABSOLUTE CROSS SECTION FOR EXCITATION OF THE \((2p^5)3p\) CONFIGURATION OF NEON BY He\(^+\) IMPACT. The open circles are present data. The closed circles are the emission cross section data of DeHeer et al, van Eck et al and Jaecks et al (Refs. 6, 8 and 9).
in good agreement with a large class of heavy ion-atom interactions.

Since this transition is optically forbidden, one expects, from qualitative results obtained by the Born approximation, that the high energy fall off in the cross section should be very rapid («1/E). In the case of proton impact, our data in fact indicate precisely this type of behavior. The behavior is not observed as dramatically for H₂⁺ impact although the cross section is definitely decreasing above 90 keV. We were not able to observe the phenomenon in He⁺ impact since our highest energy lies just above the peak of the curve.

For H⁺ and He⁺, emission cross section data of DeHeer et al, van Eck et al and Jaecks et al are shown for comparison with our results. Their data consist of the sum of three transitions from levels within the 3p configuration to levels of the 3s configuration having wavelengths of 5852, 5882 and 5945 Å. The agreement between proton data is surprisingly good in view of the fact that only three of the many possible de-excitation channels are included and since no corrections for cascade effects have been made to the emission data. It is not known if the agreement observed is merely fortuitous, or if the major de-excitation channels are indeed these three. The data of Sharpton et al would seem to imply that the latter is the case.
The agreement between He\textsuperscript{+} impact data is not as good, but within the combined experimental errors. Again, since previous experiments have indicated increasing cross sections with decreasing energy for the He\textsuperscript{+}-Ne system, it is reasonable to assume that excitation of this level may also be resulting in large angle scatter at low energy.
V. CURVE FITTING OF $(2p^5)^3s$ PEAK

As previously mentioned in Sec. III, analysis of the energy-loss location of the $(2p^5)^3s$ peak as a function of both incident ion and impact energy yielded some interesting results, indicating excitation of triplet states by He$^+$ impact at low energy. The results presented by this analysis were necessarily of a qualitative nature. In an attempt to express our results in a more quantitative nature, we have developed a curve fitting technique to extract unresolved cross sections from our experimental data. The technique has been used previously with reasonable success for analysis of Helium excitations as observed in He$^+$-He scattering$^{34}$. The method is described in detail elsewhere$^{16}$ and only a brief description of the essential elements will be given here. Basically, successful application of the technique rests on four assumptions:

1.) The energies of discrete excitations are assumed to be located at the spectroscopically determined energy values;

2.) The shape of the response of each excitation is identical to that of the elastically transmitted peak, or the resolution function;

3.) The energy loss spectral response of one excitation is unaffected by the responses of neighboring excitations, with the total response being simply additive for coincident excitations; and,
4.) All of the energy loss processes which contribute to the unresolved peak are known.

All of the above assumptions are valid for our particular experiment. Assumptions 2 and 3 have been discussed in detail elsewhere. Under these assumptions, then, each point of the inelastic energy loss spectrum can be written

\[ R(\xi_i) = n \sum_{j=1}^{\infty} \sigma_j \frac{R_e(\xi_i - \xi_j)}{R_e(\xi = 0)} \]  

(9)

where \( R(\xi_i) \) is a discrete point on the inelastic energy loss spectrum located at an energy loss \( \xi_i \), \( R_e(\xi_i - \xi_j) \) is the resolution function evaluated at \( (\xi_i - \xi_j) \) where \( \xi_j \) is the energy loss location of transition \( j \) having a cross section \( \sigma_j \); \( n \) and \( \ell \) are as defined previously. The sum is taken over all transitions which have energy losses lying within the resolution width of \( \xi_i \). Of course this particular equation assumes discrete processes and thus is valid only to energy losses which lie greater than the resolution half width below the onset of the ionization continuum.

In theory, if \( n \) discrete processes contribute to an unresolved peak, then only \( n \) points on the spectrum are required for a unique solution of Eq.9. However, due to unavoidable random noise in the data, the accuracy of an
exact solution is somewhat in doubt. Thus, to improve
the accuracy, Eq. 9 is least-squares fitted to k points
on the energy loss spectrum, where k is taken as large
as possible without including contributions from pro-
cesses not considered in the sum over j. (typically, k
was chosen to be 20 for present measurements) The cross
sections are then obtained as the least-squares parameters
of the equation and the calculated error in the parameters
gives a reasonable estimate of the goodness of fit.

The technique was applied to the 3s peak in Neon by
assuming peaks at the spectroscopic locations of the four
levels in the configuration (see Fig.2). For this case, a
fit to these four levels yielded results which, due to
their extremely small separations and due to inherent noise
in the data, possessed rather large statistical fluctua-
tions for the three triplet levels. Therefore, the results
reported here are for the sum of the triplet levels as
this number was statistically more significant. In addition,
approximately the same values were obtained by making
another approximation and fitting a two parameter equation
with peaks at 16.85 eV ($^{1}P_{1}$) and the symmetric center of
the triplets at 16.67 eV ($^{3}P_{1}$). Unfortunately this restricts
interpretation of the results since this level is also the
one which could be populated directly if Neon was not
describable by LS coupling for this configuration.
However, the individual triplet levels cannot be expected to be statistically significant since their separation approaches the energy loss uncertainty of $\pm 0.03$ eV.

The results of the least squares analysis provided a fit to better than 5% of the larger contribution in all cases. The results are presented in Figs. 9, 10 and 11 for $H^+$, $H_2^+$ and $He^+$, respectively.

Each datum point consists of approximately 12 data trials. The parameters obtained from the curve fitting for each of the trials were used to obtain a weighted average, the weight factors being the relative calculated errors in the parameters. The error bars in all cases represent an r.m.s. combination of one standard deviation obtained from the averaging procedure, together with an estimated systematic error of 25%.

Very little triplet excitation is observed for proton and $H_2^+$ impact. The maximum value for proton impact is of the order of 25% of the total excitation cross section. This is slightly larger than which would be expected by application of the Wigner spin rule. A crude comparison can be made between our data and the coefficients calculated by Fajen$^{27}$ for the singlet-triplet mixing in this configuration. In general, the first Born approximation predicts the cross section for excitation of optically
FIGURE 9

CROSS SECTIONS FOR EXCITATION OF THE SINGLET AND TRIPLET LEVELS WITHIN THE \((2p^5)3s\) CONFIGURATION BY \(H^+\) IMPACT. The open circles are data for excitation of the \(^1P_1\) level. The solid triangles are data for excitation of the sum of the triplet levels. The dashed line is our calculated estimate of the direct population of the \(^3P_1\) level due to intermediate coupling.
Figure 9

CROSS SECTION \( (10^{-18} \text{ cm}^2) \)

IMPACT ENERGY (keV)

0  40  80  120  160
FIGURE 10
CROSS SECTIONS FOR EXCITATION OF THE SINGLET AND TRIPLET LEVELS WITHIN THE $(2p^5)3s$ CONFIGURATION BY $H_2^+$ IMPACT. The open circles are data for excitation of the $^1P_1$ level. The solid triangles are data for excitation of the sum of the triplet levels.
Figure 10
FIGURE 11

CROSS SECTIONS FOR EXCITATION OF THE SINGLET AND TRIPLET LEVELS WITHIN THE \((2p^5)3s\) CONFIGURATION BY \(\text{He}^+\) IMPACT. The open circles are data for excitation of the \(^1p_1\) level. The solid triangles are data for excitation of the sum of the triplet levels.
allowed transitions between the ground state and an excited state, \(n\), by proton impact to be proportional to the square of the generalized oscillator strength,

\[
\sigma_{on} \propto |z_{on}|^2
\]  

(10)

where

\[
|z_{on}|^2 = |\int \psi_0^* \psi_n \, d\vec{r}|^2
\]  

(11)

\(\psi_0\) and \(\psi_n\) are the wavefunctions of the ground and excited states, respectively and \(V\) is the interaction potential. We have seen that the wavefunction \(\psi_n\) can be written as a linear combination of LS basis functions and Eq.11 can therefore be rewritten as

\[
|z_{on}| = |\int \psi_0^* V(\alpha \phi^1P_1 + \beta \phi^3P_1) \, d\vec{r}| \quad (12)
\]

for the 16.85 eV peak (1s\(_2\)), and as

\[
|z_{on}'| = |\int \psi_0^* V(-\beta \phi^1P_1 + \alpha \phi^3P_1) \, d\vec{r}| \quad (13)
\]

for the 16.67 eV peak (1s\(_4\)). Now, since the matrix elements connecting the \(\phi^3P_1\) wavefunction with the ground state vanishes and since the interaction potential re-
mains the same for excitation of either state, we can write, to first order, the relative contributions of singlet-triplet cross sections,

\[
\frac{\sigma_{on'}}{\sigma_{on}} = \frac{|z_{on'}|^2}{|z_{on}|^2} = \frac{\beta^2 |\int_0^1 \psi_0^* \phi(1P_1) d\tau|^2}{\alpha^2 |\int_0^1 \psi_0^* \phi(1P_1) d\tau|^2}
\]

or,

\[
\sigma_{on'} = \frac{\beta^2}{\alpha^2} \sigma_{on}
\]

Therefore, using the calculated results of Fajen\textsuperscript{27}, the cross section for direct population of the triplet level should be

\[
\sigma_{on'} \approx 0.076 \sigma_{on}
\]

This relation has been applied to our data to calculate a cross section curve for excitation of the \(3P_1\) level, which is plotted in Fig.9. Agreement is remarkably good at energies above 80 keV. In the range from 20-80 keV our data show a slightly higher cross section with a peaked structure. However, within the error of the measurement and the calculation, it is impossible to make any definite statements.
The lack of triplet excitation by \( \text{H}_2^+ \) is surprising. Since this ion carries an electron, excitation of triplet levels should occur by electron exchange. One is tempted to conclude that exchange excitation does not occur very significantly for \( \text{H}_2^+ \) bombardment. However, van den Bos et al.\(^{35}\) and Rudd\(^{29}\) have observed triplet excitation of Helium by \( \text{H}_2^+ \) impact, with cross sections comparable to those for excitation for the singlet states. A possible explanation for this apparent discrepancy is that sufficient distortion of the molecular structure occurs during the collision that the \( \text{H}_2 \) ion dissociates. Our experiment would not detect such a result since analysis is done on the primary particle. The experiment of van den Bos would not be sensitive to this process either, since only the optical emission is studied, while all of the incident beam is collected in a Faraday cup, without mass analysis.

Helium ion impact thus provided the only data in which significant triplet excitation occurred. To the authors' knowledge, there are no other experimental data with which to compare these results.
VI. DISCUSSION

At present, the authors' know of no theoretical calculations for this system with which to compare present results. However, good approximate wave functions are available for Neon and the problem is soluble in principle. The data presented here are the first excitation measurements using the technique of heavy-ion energy-loss spectrometry for which data obtained by the optical method have been available for comparison. Agreement, as we have seen, is not good for excitation of the \((2p^5)3s\) configuration. Part of the discrepancy is explainable by the differences in the measured quantities and the absolute numbers (except for the case of \(He^+\) impact at very low energies) are within the combined errors of the two methods. The differences in shape are disturbing, however resolution of this problem must await a more detailed analysis of the cross section function as a function of scattering angle. Agreement between data for the excitation of the \((2p^5)3p\) configuration was surprisingly good. On balance, in view of the basic differences between the two methods, the results of this comparison are not totally unsatisfactory.

Analysis of the relative population of singlet-triplet levels within the \(3s\) configuration, while yielding values with relatively large experimental uncertainties,
has been able to illustrate some qualitative aspects of the heavy ion-Neon scattering process. The proton impact data are in agreement with both the Wigner spin rule and the calculated LS purity of the 3s level, as expected. The He$^+$ data indicate that triplet excitation by electron exchange is a significant process in Neon at low velocities and cannot be excluded from any theoretical attempts to explain scattering phenomena in the energy range of the present experiment.

The data for triplet excitation by H$_2^+$, together with the data of Rudd$^{29}$ and van den Bos et al.$^{35}$ imply that electron exchange may occur only with concurrent dissociation of the H$_2$ molecule. Further experimental investigation of this system by actually measuring cross sections for simultaneous electron exchange-dissociation is suggested and should yield interesting information.
VII. APPENDICES

A. Apparatus Modifications - Data Acquisition

I. INTRODUCTION

This study was performed using the University of Missouri - Rolla 250 keV heavy-ion energy-loss spectrometer. Modifications have been made to enable more precise measurements to be made of the energy losses occurring in inelastic ion-atom collisions. This improvement has permitted estimates to be made of the relative contributions of singlet and triplet excitations in the \((2p^5)3s\) configuration of Neon as a function of both impact energy and projectile type.

In this section, the apparatus will be described briefly as background material for a more detailed description of the modifications which have been made. Suggestions are made concerning a number of additional experiments which are now possible.

II. APPARATUS

A schematic diagram of the apparatus is shown in Fig. Al. The \(H, H_2\) and He ions used in this study were formed in a Colutron\(^{14}\) ion source by bombarding a mixture of water vapor and He and Ar with electrons having a maximum energy of 40eV. The ions are extracted and focused by a

†This section has been accepted in part for publication in The Review of Scientific Instruments, and will appear in the Feb. 1972 issue of that journal.
FIGURE A1

SCHEMATIC DIAGRAM OF THE UMR HEAVY-ION ENERGY-LOSS SPECTROMETER.
three element einsel lens and accelerated to the desired energy by an acceleration column of the constant voltage gradient type. The beam is then steered electrostatically into a differentially pumped scattering chamber containing the Neon gas.

After the beam emerges from the scattering chamber, it is magnetically momentum analyzed to obtain the particular ion species of interest. The beam is then decelerated to a low, well defined energy. The ions are then energy analyzed by a $127^\circ$ electrostatic analyzer. Those ions which satisfy the energy requirements established by the analyzer plate voltages are detected by an 18 stage EMI particle multiplier. The output signal is then routed to the appropriate instrumentation for processing.

Spectra are obtained from the system by slowly varying the potential of the accelerator relative to that of the decelerator. That is, if we assume the analyzer is set to detect ions having an energy of 2 keV, then when gas is in the chamber and the potential difference between the two terminals is 2 kV, only ions which have not undergone a collision or which have been scattered elastically will be detected. If we now increase the potential difference slightly, only those ions which have lost an amount of energy equal to the increased potential difference will successfully traverse the analyzer and be detected. The original
beam, unscattered and elastically scattered particles, will now have an energy greater than 2 keV and will not be detected. By continuously increasing the potential difference, an energy loss spectrum is obtained. Whenever the added voltage corresponds to an allowed process of the projectile-target system, a peak is detected in the spectrum.

In actual practice, the high voltage, $V_H$, is applied first to the decelerator terminal. The offset ($V_o$) and sweep ($\Delta V$) voltages are then added in series and the total voltage, $V_a = V_H + V_o + \Delta V$, is applied to the accelerator terminal. This has the experimental advantage of removing any difficulties from high voltage power supply drift and ripple since both terminals see the same effects. The absolute energy of the beam as seen by the detection apparatus remains well defined by the precision offset and sweep power supplies.

The data are defined, then, as pairs of points, $(\xi, I)$, where $\xi$ is the energy loss as measured from the most probable value of the unscattered beam and $I$ is a measure of the detected current.

The energy loss scale in this method is established by the sweep power supply, $\Delta V$. However, since all detection apparatus and this power supply are located at high voltage, some means had to be devised to both control and measure the value of $\Delta V$ and to measure the detected current from
ground potential.

Previously\textsuperscript{11}, this was accomplished in the following manner. The sweep power supply was resistance programmed by a potentiometer located at the high voltage terminal. This potentiometer was varied from ground potential by means of a nylon rod to which another potentiometer was attached at the ground end. A small power supply across the potentiometer located at ground potential then provided a voltage proportional (1:10) to the output of $\Delta V$. The relative current was detected by means of a picoammeter whose analog output was used to drive a servo amplifier system which turned a nylon rod. A potentiometer was attached to the ground end of this rod and provided another proportional voltage. Spectra were then recorded on an X-Y recorder using these voltages as the X and Y axes, respectively.

In this method, the accuracy of the energy loss scale is subject to a number of possible error sources such as calibration of the two potentiometers, mechanical backlash, recorder deadband and human errors in reading the graphs. In order to improve the precision of the energy loss scale, the apparatus depicted in Fig. A2 was developed.

The primary change is that the function of $\Delta V$ has been assumed by a digitally programmable voltage calibrator,\textsuperscript{36} whose output state is specified by the voltage programmer.
FIGURE A2

SCHEMATIC DIAGRAM OF THE DATA ACQUISITION SYSTEM. The ΔV fiber optics bundle contains 28 data channels.
Figure A2
This power supply can be incremented in equal steps, ranging in size from 0.1μV to 100V per step. Thus, the energy loss scale is established to the precision of the power supply since its output voltage is known in digital form from the voltage programmer. The original sweep voltage, now defined as \( \Delta V_s \), is retained as an aid in beam tune-up and is turned to zero when actual data is taken.

Since the energy loss scale is now established by equal steps and since the apparatus may be held at any step for a defined length of time, counting techniques may be utilized for detection of beam current.

The energy loss spectra data pairs are obtained at ground potential by the use of optical telemetry. The energy loss is presented in 7 decades of 1248 BCD logic from the voltage programmer, which drives a light-emitting diode(LED) matrix. The signal is detected at ground potential by a similar matrix consisting of photo-transistors.

The current is measured at ground potential by a digital counter operating in a frequency mode. The input signal to the counter is derived from a photomultiplier tube at ground potential, whose input consists of light pulses from a LED located at the high voltage terminal. This LED is driven by discriminator output pulses from a pulse-amplifier-discriminator(PAD). The input to the
PAD is determined by the beam intensity.

If the beam intensity is sufficiently low that counting techniques can be employed, the output of the particle multiplier is used directly. If, however, the beam intensity is high, such that the particle multiplier dead time prohibits counting, the current is measured by a picoammeter whose analog output is converted by a voltage-to-frequency converter into pulses whose frequency is proportional to the detected current. These pulses are then used as the input to the PAD.

The data are then transmitted, together with pertinent manual data (e.g. graph number, electrometer range, etc.) to a coupler which formats the data and transmits it serially to a paper tape punch for recording.

An analog signal is derived from the current measurement at ground potential by a diode pump circuit for use as the Y axis of an X-Y recorder. This signal is then plotted versus time as a visual aid to the operators.
III. VOLTAGE PROGRAMMER

The output level of the D-A converter (ΔV) is determined by the state of the voltage programmer which is shown schematically in Fig. A3. The programmer serves three basic functions:

1) It provides seven decades of 1248 BCD coding in negative logic levels compatible with the D-A converter.
2) It drives a LED matrix for transmission of the data to ground potential, and
3) It provides a visual readout of the voltage by means of a Nixie display.

The voltage step size is determined by the decade selector switch and the voltage range switch (the latter is not shown). A stepping pulse produced by the counter at ground potential drives a LED which sends an optical pulse through a fiber optics channel to the step control located in the decelerator. The pulse is detected by a photo-transistor and transformed into a logic level pulse. This pulse drives the one-shot module which is used basically as a pulse stretcher-inverter in this application. The output from the one-shot is directed to the appropriate decade counter module which simultaneously drives the Nixie display, diode drivers and inverters. The decade counter modules are set by a high logic level and count when the input steps to low level. Overflow occurs
All logic modules are of the DEC\textsuperscript{37} type.
Q1=LS400 photo-transistor; Q2=2n2219; D1=1n483
PROGRAMMING BUS TO D-A CONVERTER (ΔV)

INVERTER 1248
NIXIE DISPLAY
LAMP DRIVER
DECADE COUNTER 10^0

INVERTER 1248
NIXIE DISPLAY
LAMP DRIVER
DECADE COUNTER 10^1

INVERTER 1248
NIXIE DISPLAY
LAMP DRIVER
DECADE COUNTER 10^6

TO DECADE 10^2

FROM DECADE 10^{5,8}

STEP CONTROL +5V

ONE SHOT

Figure A3
through the use of the NAND gates. When the inverted "8" bit of the preceeding decade goes low, the NAND gate output provides a high level to set the decade counter module. When the "8" bit then goes high on overflow, the output of the NAND gate goes low, initiating the count. All of the modules are of the DEC\textsuperscript{37} type.
IV. OPTICAL TELEMETRY

The optical telemetry techniques used to obtain data from the high voltage terminal have been used previously\textsuperscript{38} for physical isolation of detection and measurement apparatus. In the present experiment, two types of signals are transmitted. The energy loss scale requires the transmission of low frequency logic level signals, while the relative current requires the transmission of high frequency (~300kHz) pulses.

Monsanto ME-7 LED's are used for the logic signals. These diodes emit 0.5 mW of power centered upon a wavelength of 0.9\textmu m. The current transmission uses a Monsanto MV-50 which emits at a peak wavelength of 0.65\textmu m. Both types have a pulse width of 1 nsec.

The output of these diodes is transmitted to ground potential through 1/16 in.-diam x 4 ft non-coherent fiber optics channels. These light rods have successfully maintained a potential difference of >200kV without breakdown.

The digital signals are detected at ground potential by low speed silicon photo-transistors (LS-400). These transistors have a dark current of 25 nA and a light current of 3 mA for an incident power of 9 mW/cm\textsuperscript{2}. Their speed is limited primarily by their slow (15 \mu sec) fall
time.

The current pulses are detected by means of an RCA type 931 photomultiplier. The system has been tested at repetition rates of up to 1 MHz and found to be linear up to that frequency.
V. METHOD OF OPERATION

Control of the system is achieved through use of the internal timing of the counter. A typical timing diagram is illustrated in Fig. A4 for a sample time of 0.1 sec.

Measurement occurs during the period when the gate is open, the duration of which is determined by one cycle of the internal clock. Upon termination of the measurement, a record command is generated and the coupler transfers the (\(\xi, I\)) data pair to paper tape. After 70 msec has been allowed for data transfer, a step command is generated. This command drives the stepping diode which transmits an optical pulse to the step control at high voltage and advances the D-A converter one unit.

The system is then ready for another measurement when the sample rate multivibrator returns to low level after its preset time. This multivibrator is initialized upon gate closure and inhibits gate opening until it returns to its stable state. The duration of the pulse is variable from 170 msec to infinity. The power supply is thus allowed a minimum of 100 msec to settle to its new value. After the end of the multivibrator pulse, the gate is free to open on the first positive going clock pulse.

All of the data for this study were taken using the picoammeter as the current measurement device. A data
FIGURE A4

TIMING DIAGRAM. Pulse heights are not shown to actual relative scale.
Figure A4
spectrum is obtained by setting the analyzer plate voltages such that the unscattered peak is detected with $\Delta V_s$ set at approximately 3V. The sweep voltage is then set equal to zero and $\Delta V$ is stepped continuously in units of 0.1 or 0.01V. Once the elastically scattered peak has been recorded, the picoammeter gain is increased by a factor of 100 or 1000 and the inelastic portion of the spectrum is recorded.

The energy loss is determined by locating the voltage corresponding to the most probable value of the elastic peak, by fitting a second order equation to 11 points centered around the maximum value of the peak. This voltage is then used as the zero reference of the energy loss scale. The inelastic data are then converted to energy losses by subtracting the value of the peak voltage from the recorded voltage for each point. The current values are converted to differential cross sections by computer elimination of experimental parameters and subtraction of the background as obtained with no gas in the target chamber. In this way, a paper tape consisting of energy loss - differential cross section data pairs is generated, for later computations.
VI. DISCUSSION

The apparatus described above has succeeded in defining the energy loss scale to a precision of \( \pm 0.03 \) eV. The major source of the remaining uncertainty is believed to be due to small changes in the initial energy of the beam as it emerges from the ion source. The source of this difficulty is apparently due to variations in contact potential within the source, and modifications are currently in progress to attempt to eliminate this problem.

The system has proven itself to be a very efficient data collection device. Over 1000 data runs were collected for purposes of this project and computer analysis has drastically shortened the time for data reduction over that required by previous graphical techniques. The savings from this aspect alone are obvious.

In conclusion, the system's versatility has been expanded by the installation of the new data collection system. Several new experiments suggest themselves as a result of this expanded capability. For example, it is now possible to do coincidence experiments between photons emitted from the target particle and the projectile which caused the transition. This would be a valuable method to improve the energy resolution of the system and yet retain the absolute nature of the quantitative cross
sections obtained. The system also permits measurements to be made at lower beam intensities, thus making measurements of doubly differential (angle and energy loss) cross sections feasible.
B. Curve Fitting of Energy Loss Data

Under the assumptions given in Sec.V of this paper, we can write an expression for any point on the inelastic portion of an energy loss spectrum as

\[ R_i = C \sum_{j=1}^{m} \sigma_{ij} \]  

where \( R_i \) is the relative inelastic current at \( \xi = \xi_i \),

\[ C = n \xi R_0(\xi = 0) \]  

where the terms on the right are as defined previously, and

\[ a_{ij} = \frac{R_0(\xi_i - \xi_j)}{R_0(\xi = 0)} \]  

\( R_0(\xi) \) being the resolution function and \( \xi_i \) the energy loss corresponding to the discrete process having the cross section \( \sigma_{ij} \). Although only \( m \) values of \( R_i \) are needed for a unique solution of Eq.B1, better results are obtained if the equation is least-squares fitted to as many points as possible. If we assume that all of the error can be associated with the magnitude of the relative current, \( R_i \), and that the energy loss is known exactly, we can obtain a least-squares solution for \( k \) points on the spectrum. Each of the cross sections can be found from an equation of the form
There are m such equations and simultaneous solution yields the cross section

\[
\sigma_j = \frac{\begin{vmatrix}
\sum_{i} a_{il}^2 & \frac{1}{C} \sum_{i} R_i a_{il} & \cdots & \sum_{i} a_{il} a_{im} \\
\cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
\sum_{i} a_{il} a_{im} & \frac{1}{C} \sum_{i} R_i a_{im} & \cdots & \sum_{i} a_{im}^2 
\end{vmatrix}}{\begin{vmatrix}
\sum_{i} a_{il}^2 & \sum_{i} a_{il} a_{ij} & \cdots & \sum_{i} a_{il} a_{im} \\
\cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
\sum_{i} a_{il} a_{im} & \sum_{i} a_{im} a_{ij} & \cdots & \sum_{i} a_{im}^2 
\end{vmatrix}}
\]

The error in the parameters (cross sections) can be calculated from the k contributions to the error due to the separate R_i's. The error in \(\sigma_j\) is

\[
s_{\sigma_j} = \sqrt{\sum_{i} \left( \frac{\partial \sigma_j}{\partial R_i} \right)^2 s_{R_i}^2}
\]

where

\[
s_R = \sqrt{\sum_{i} (\delta R_i^2)/(k-2)}
\]
The error can be easily evaluated from these equations for a given number of peaks. All of the required sums are available as output from the computer program which performs the solution.

An example of the fit obtained by this procedure for the data of the present study is shown in Fig. B1. The data presented are for the case He$^+ \rightarrow$Ne at an impact energy of 60 keV. The cross sections obtained for this particular run were: $\sigma(3P_J) = 3.17 \times 10^{-18}$ cm$^2$ and $\sigma(1P_1) = 1.27 \times 10^{-18}$ cm$^2$. The upper curve shows the raw data and the individual peaks located at 16.67 and 16.85 eV. The lower curve shows the raw data and the result of the addition of the two peaks. For this case,

$$\frac{s_{\sigma_1}}{s_{\sigma_2}} = 1.5 \times 10^{-19} \text{ cm}^2 \quad (B8)$$

The error calculated in the above procedure, while not an actual measure of the absolute accuracy of the measurements, due to shifts in the energy scale, does give an estimate of the goodness of fit. This, in turn, can be used as an estimate of the reliability of each measurement and a weighted average is made using the calculated errors in the least squares parameters as the basis for the assignment of relative weights.

In a further attempt to assign some reliability to
FIGURE B1

COMPARISON OF CURVE FITTING RESULTS WITH DATA. The data presented here is for $\text{He}^+$ impact on Neon at an energy of 60 keV. The upper curve consists of a plot of raw differential cross section data. The two smaller peaks are the results of placing peaks at the spectroscopic locations of the $^1P_1$ level and the symmetric center of the triplets ($^3P_1$ level), each with the shape of the resolution curve and relative heights as obtained from the curve fitting procedure. The lower curve shows a comparison of the sum of the two smaller peaks with the raw differential data.
Figure B1

The graph shows the energy loss, $\xi$, (eV) plotted against $d\sigma/d\xi$, normalized to $10^{-18}$ cm$^2$/atom-eV. The lines represent different processes:

- $d\sigma/d\xi$ (DATA)
- $d\sigma/d\xi (\Sigma^3P_J)$
- $d\sigma/d\xi (^1P_1)$

The data points and smooth curves illustrate the behavior of these processes across the energy loss spectrum.
the technique, we have devised another method for obtaining approximate ratios for comparison with the results obtained from the curve fitting.

Since, for present data, the energy loss peaks are so closely spaced, no structure appears in the convoluted peak. Hence, we have written a computer program which takes a resolution function (elastic peak) as input and performs a convolution of the inelastic structure using varying relative ratios for contributions from the contributing processes. The peak of the structure thus obtained is located in the same manner as for actual data. (11 point fit to a second order equation)

The results obtained for a typical resolution curve are shown in Fig.B2. The relative triplet-singlet ratios are plotted versus the location of the peak. Data are shown for the case in which one peak is placed at the symmetric center of the triplets (16.67eV) and for the case in which peaks are placed at all of the triplet levels, each peak containing one-third of the sum. It can be seen that the differences between the results obtained when using two peaks from those when using four peaks are negligible, justifying our previous assumption in Sec.V.

Data obtained from such curves have been used to de-
FIGURE B2

RELATIVE TRIPLET-SINGLET RATIO VS PEAK LOCATION. Computer generated convoluted peaks using actual resolution functions have been obtained with varying relative ratios of singlet-triplet heights. The peak location is then found using the same procedure as that for obtaining energy loss locations in the data. The crosses are the data obtained by using two peaks (\(^1P_1\) at 16.85 eV and \(^3P_1\) at 16.67 eV) in the convolution. The solid circles are the data obtained by using four peaks, located at the energies corresponding to the four levels of the configuration, in the convolution. The data for four peaks has been displaced 0.01 eV to the right for clarity.
Figure B2
termine the relative ratio of triplet-singlet cross sections for each ion-energy data set, using the average energy loss obtained from each set. The results obtained from the two methods are in reasonable agreement with the larger contribution in all cases. Whenever the smaller contribution approaches a value below 10% of the total, however, the statistical fluctuations in the smaller value become large, indicating that, in these cases, only an upper limit can be assigned with certainty.

It should be noted that the technique is not an application of deconvolution since the exact form of the resolution function is known in all cases. It requires only that all processes contributing to a specific peak be included in the analysis. Of course, due to noise in the data, limitations are imposed as to the minimum separation of the peaks which can be resolved. From our results, it appears that, at a separation of 0.18 eV, noise and random energy shifts result in error in the estimation of contributions which amount to less than 10% of the peak height. However, there are many additional data systems for which the separations are larger than that for Neon, but which are still not completely resolved by the energy-loss spectrometer. This technique should aid in analysis of such data.
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IX. VITA

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