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The Response of the $1P^0$ Resonance Near $n=3$ in the H^- Continuum to External Electric Fields

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THE RESPONSE OF THE $1p\sigma$ RESONANCE NEAR $n=3$ IN THE H^- CONTINUUM TO EXTERNAL ELECTRIC FIELDS

Stanley Cohen

Abstract

The response to external electric fields of the $1p\sigma$ resonance in the H^- photodetachment continuum below the $n=3$ hydrogenic excitation threshold is investigated. Using the relativistic ($\beta = 0.806$) 650 MeV H^- beam at the Clinton P. Anderson Meson Physics Facility (LAMPF) in Los Alamos, the fourth harmonic (2.66 nm) of a Nd:YAG laser is Doppler shifted to provide a continuously tunable photon beam in the rest frame of the ions. The magnetic field from pulsed Helmholtz coils, surrounding the photon- H^- interaction point provides a Lorentz-transformed barycentric electric field.

Relative total photodetachment cross sections were measured as a function of photon energy and electric field. The resulting spectra were fit to a Fano line shape,

$$\sigma(\epsilon) = \sigma_a \frac{(q + \epsilon)^2}{1 + \epsilon^2} + \sigma_b,$$

with Γ being the full width at half maximum (FWHM) of the resonance, E_0 its center, σ_a the resonant cross section, σ_b the nonresonant cross section and q the line profile index.

Within experimental uncertainties, the values of E_0 , q and the effective strength, with no external field, obtained by the current experiment, agree with the a previous measurement by Hamm et al.²¹ The present data shows Γ to be 39 ± 2 meV as compared to the previous measured value of 27.5 ± 0.8 meV. This discrepancy is discussed. All of the fitted parameters are corrected for the 0.007 eV energy resolution of the experimental apparatus.

As the magnitude of the external field was increased, there was no observed shift in E_0 , until quenching occurred at a field strength of 2.36 MV/cm. The effective strength of the resonant state appears to decrease linearly with increasing field. The line shape index, q , is constant within statistical uncertainty, until the resonance disappears. There is, also, evidence that the resonance may narrow at fields below 1.25 MV/cm. It then broadens at higher fields before quenching.

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Background

Although the negative hydrogen ion (H^-) is a simple atomic system, describing its behavior quantum mechanically is not a trivial exercise. Experimental data from this three-body Coulomb system is viewed with great interest since H^- can be used as a test bed for checking the validity of theoretical models in atomic and molecular physics. Past reports of observations of its ionization threshold behavior and resonant structure have provided stimuli for theoretical investigations of short range electron correlation effects and bound states in the continuum. Risley^{1,2} provides comprehensive historic background of experimental investigations of the H^- ion. Current theoretical workers include Lin,^{3,4,5} Ho,⁶ Greene,^{7,8} and Callaway.^{9,10}

The H^- ion has only one state whose energy is below the first ionization level of the system.^{11,12} This is, strictly speaking the only bound state of the system. Early attempts to calculate the bound state energy for H^- used identical radial hydrogenic wave functions for both of the ion's electrons and predicted no bound states. Wave functions with different scaling factors were required to produce a positive value for the binding energy for the second electron.¹³ The H^- ion can be characterized as a polarized hydrogen atom with a second electron loosely bound to it.¹ A widely accepted value

for the H^- binding energy is 0.754212 eV, calculated by Perkeris¹⁴ in 1962.

Excited states (resonances) of the ion are doubly excited and autoionizing (the Auger effect), that is, the H^0 core of the system is also excited and an electron is eventually spontaneously ejected leaving atomic hydrogen. The $3p^e$ (triplet P even parity) state is the only doubly excited state that is not autoionizing.¹⁵ Further references to bound states of H^- will include these doubly excited states.

Resonances can be seen through electron-hydrogen scattering, eq 1.1¹⁶ or by observing the photodetachment spectrum of H^- , eq 1.2:

and

The 800 MeV proton linear accelerator at the Clinton P. Anderson Meson Physics Facility (LAMPF) at Los Alamos permits high resolution photodetachment studies using the linac's H^- beam. Experimental details of this work will be discussed later.

Experiments at LAMPF have identified the Feshbach and shape resonances near the hydrogenic $n=2$ threshold,¹⁷ documented the response of these resonances to strong

external electric fields 18,19,20 and identified recursions of the $1p\sigma$ closed channel resonances below $n=3$.²¹ Reviews of these experiments have been published by Bryant,²² Bryant et al.,^{19,23} and Smith et al..²⁴ This present work will report observations of the response of the resonant states near $n=3$ to moderate and strong external electric fields.

Resonances are classified as closed channel (or Feshbach) and open channel. Feshbach resonances, first predicted using the Feshbach projection operator formalism,^{25,26,27} occur just below the energy threshold of a hydrogenic excited state. This state will exist when the interaction between the extra electron and the excited hydrogen core is strong enough to support a bound state. If there are terms in the Hamiltonian that couple the bound state to the continuum of the atomic core and a free electron, the state will be unstable.

In photodetachment, if the energy of the incident photon is high enough to produce an excited hydrogen core, there may be enough energy to produce a potential with a barrier and an inner well of a shape that can support a bound state. This bound state does not modify the quantum numbers of the excited hydrogenic core and occurs above the excitation threshold of the core ^{28,29}.

Fano³⁰ was forced to discard the assumption of independent electrons in motion around the nucleus. If

accurate predictions of the behavior of multi-electron atoms were to be made, correlated electronic motion must be assumed. Angular momentum states for these electrons could not be defined as if the motion of the two electrons were uncoupled. Electronic states need to be characterized as a linear combination of independent particle states. Cooper, Fano, Prata³¹ first used "+" and "-" representations to explain the doubly excited states in He observed by Madden and Codding³². These symmetric hydrogenic wave functions can be represented schematically as

$$"+" = 2anp + 2pns$$

and

$$"- " = 2anp - 2pns,$$

where "s" and "p" are the orbital angular momentum states of the electrons and "n" is the principal quantum number of the configuration. More recently this formalism has been extended using group theoretical methods to classify correlated electron states³³.

Lin^{3,34} calculated a pair of hyperspherical potentials, based upon the "+" and "-" configuration states of Cooper et al..³¹ Lin's technique, expanding upon that of Macek,³⁵ involves transforming a three-body problem into a quasi-two-body one by creating a hyperspherical coordinate system to describe the relative locations of the two electrons from the nucleus. In this coordinate system the

Figure 1.1 Hyperspherical potentials.
 Field-free potential curves of H^- converging to $H(n=2)$ limits. The + and - $1p0$ curves support the shape and Feshbach resonances respectively.
 (from C.D. Lin, Phys Rev A 14, p30 (1976))

distances from the nucleus r_1 and r_2 are replaced by the hyperradius $R = (r_1^2 + r_2^2)^{1/2}$ and a hyperangle $\alpha = \tan^{-1}(r_2/r_1)$. The "+" and "-" potentials for the $1p$ states of H^- near $n=2$ are shown in Fig. 1.1.

Resonances near $n=2$ in External Fields

Recently, attention has turned to the motion of correlated electrons in external electric fields. Prompted by the attempt, with negative results, by Ott et al.³⁶ to observe the shape resonance in a high temperature hydrogen plasma, and the actual observation by Bryant et al. at LAMPF.¹⁸ Wendoloski and Reinhardt³⁷ calculated the response of the resonances near $n=2$ in an external electric field. Since a photon carries only one unit of angular momentum, only the P state is accessible through single photon excitation. The external field allows access to other angular momentum states.³⁸ The presumption was that external fields would have a tendency to quench the resonance as more angular momentum states were made accessible. The failure of Ott to see the shape resonance was assumed to have resulted of quenching from local microfields in the plasma. The response of the Feshbach and shape resonances near the hydrogenic $n=2$ threshold to external electric fields was observed by Gram, et al.¹⁸ and Bryant et al..¹⁹

More detailed measurements of the Feshbach resonance

revealed a triplet splitting in an external field. Two outer components could be attributed to a linear Stark shift and the center exhibited a quadratic Stark shift. This resonance quenched at much lower external fields than did the shape. The shape resonance became broader (its energy FWHM became wider) at increasing electric fields, see figure 1.2(a) and 1.2(b) below. By using light polarized either parallel or perpendicular to the external field, the outer states were observed to correspond to the magnetic quantum state of $M=0$ and the center to $|M|=1$. Butterfield²⁰ discusses details of the Stark broadening of these resonant states.

Motivated by the experimental results outlined above, Lin⁵ calculated a family of hyperspherical potentials for the correlated electronic motion near $n=2$ for a set of increasing values of external fields. The potentials associated with the shape possess a repulsive barrier even at low external fields. The stability of the shape resonance could be attributed to the tunneling through the potential barrier by the trapped second electron. Calculated hyperspherical potentials for the $1s\epsilon$, $1p\sigma(-)$ and $1p\sigma(+)$ are shown in figures 1.3(a), 1.3(b) and 1.3(c) respectively.

Figure 1.2 The response of the Feshbach and shape resonances to an external electric field.
(from H.C. Bryant et al., Phys Rev A 27, 6, p2889 (1983))

(a) The variation of the zero-field $1S^+$ potential curve with electric fields. The electric fields are given in units of kV/cm. (b) Similar to (a) but for the zero-field $1P^+$ (-) curve. The two horizontal arrows indicate the position of field-free resonances.

FIG. 3. Similar to Fig. 2 but for the field-free $1P^+$ (+) curve. The electric fields are given in units of MV/cm.

Resonances near $n=3$

The results presented here are the continuation of the investigations of the only other observations of the resonant structure in the H^- photodetachment spectrum near $n=3$ reported by Hamm, et al.,²¹ This present work is concerned principally with the response of the $n=3$ states to external electric fields.

Observations of the states near $n=3$ were reported before by McGowan,³⁹ Williams⁴⁰ and others in the context of e^-H^0 scattering. The experimental technique used by Hamm et al.,²¹ which is essentially the same as used here, has an energy resolution (6 meV) approximately ten times that of Williams⁴⁴ (60 meV). The results of these scattering experiments are shown in Fig 1.4. Electron hydrogen scattering provides access to all angular momentum states, seen by comparing Fig 1.4 with Fig 1.6.

Gailitis and Damburg^{41,42} had proposed that the resonances that lie below hydrogenic thresholds above $n=2$, exponentially approach the threshold in the following way,

$$\frac{E_t - E_n}{E_t - E_{n+1}} = \frac{\Gamma_n}{\Gamma_{n+1}} = \exp(2\pi / (\text{Im} \sqrt{a + \frac{1}{2}})) \quad (1.3)$$

where $(E_t - E_n)$ is the distance in energy of the n th resonance from the threshold. Γ_n is energy width of the

n th state, and a is the eigenvalue of the matrix $l(l+1) + \alpha$ constructed from coefficients of centrifugal and dipole terms in close coupling equations between channels opening under the $n=3$ threshold. The coefficient a is the strength of the long range potential $V(r) \rightarrow -a/2r^2$. The threshold behavior differs depending on the sign of $a - \frac{1}{2}$. For $a > \frac{1}{2}$ an infinite number of bound states below threshold are predicted, the number will be finite if $a \leq \frac{1}{2}$.^{43,44,45} The constant a is in effect the strength of the long range dipole potential, $V(r)$, between the polarized hydrogen atom and the second electron of H^- . If the dipole interaction is sufficiently strong relative to the total angular momentum, then there will exist an infinite series of resonances (of the same L and S) just below a hydrogenic excitation threshold⁴⁶.

Gailitis⁴⁷ tabulated the locations of the H^- resonances converging to the hydrogenic $n=3$ threshold.

Herrick⁴⁸, Kellman and Herrick^{49,50}, Herrick et al.⁵¹, Gailitis,⁵² Read⁵³ have searched for symmetries that could predict the positions of resonant states. Herrick et al.⁵¹ have used a group theoretic approach to classify resonant states.

The 2S state total excitation cross section is shown as a function of incident electron energy. The present experimental values (....) are compared with the experimental values of Koschmieder *et al* (1973) (— · —), Oed (1971) (—) and Kauppila *et al* (1970) (—) and with composite (see text) close-coupling predicted values (—).

Figure 1.4 The 2S state excitation of atomic hydrogen from J.F. Williams, J. Phys B 9 p1519 (1976)

A number of techniques have been used to calculate energies of the H^- bound states. Ho and Callaway⁵⁴ use a method of complex-coordinate rotation. To uncover resonances the Hamiltonian $H(\theta)$ operator is rotated in the complex plane using the transformation $r \rightarrow r e^{i\theta}$, $\theta > 0$ and is real. Bound states are invariant under this transformation, the continuum rotates by 2θ into the lower complex plane. Isolated complex eigenvalues show up as poles in the lower complex plane and can be associated with a resonance⁵⁵. Ho⁵⁶ used this method to calculate the locations of the resonances observed by Hamm et al..²¹ Agreement for both the location and width of the resonances was quite good, see Table 1.1. The complex coordinate method is reviewed by Ho⁵⁷.

Table 1.1 Comparison of various predicted parameters of the 1p0 dip of H^- below $n=3$ and the experimental results of Hamm et al..²¹

Investigator(s)	E_0	width (see Chapt 4)
Morgan et al. ⁵⁸	12.6586 eV	0.0329 eV
Oberoi ⁵⁹	12.6605	--
Chung ⁶⁰	12.6602	--
Greene ⁶¹	12.6687	--
Ho ⁵⁷	12.6476	0.0318
Hamm et al. ²¹	12.650 $\pm$ 0.004	0.0275 $\pm$ 0.0008

Greene⁶⁰ has been able to confirm the experimental observations of Hamm et al.²¹ using a combined hyperspherical coordinate and semiempirical quantum defect theoretical (QDT) approach. The experimental data of Hamm et al. is compared to Greene in Fig. 1.5.

To date there has been little theoretical exploration of the effects of an external electric field on the bound states below $n=3$.

Strongly correlated electronic motion was indicated by the surprising resistance to quenching by external electric fields of the shape resonance above the $n=2$ threshold. It is logical to extend these electric field studies to the region near $n=3$ in an attempt to increase our understanding of this effect. A systematic investigation of the effect of increasingly intense external electric fields on the $1p\sigma$ resonance below $n=3$ was carried out. Chapter 2 reviews the experimental method which was similar to previous experiments in this series. The reader will find details of the mechanics of the investigative technique and data analysis in Chapters 3 and 4.

Summary of the Current Investigation

In brief, the relativistic ($\beta = 0.806$) 650 MeV H^- beam at the Clinton P. Anderson Meson Physics Facility (LAMPF) in Los Alamos was used to Doppler shift the fourth harmonic (2.66 nm) of a Nd:YAG laser to provide a continuously tunable photon beam in the rest frame of the ions. The

magnetic field from pulsed Helmholtz coils, surrounding the photon-H⁻ interaction point provides a Lorentz transformed barycentric electric field.

Relative total photodetachment cross sections were measured as a function of photon energy and electric field. The resulting spectra were fit to a Fano line shape,

$$\sigma(\epsilon) = \sigma_a \frac{(q + \epsilon)^2}{1 + \epsilon^2} + \sigma_b, \quad (1.4)$$

where $\epsilon = (E - E_0)/(\Gamma/2)$ with Γ being the FWHM of the resonance, E_0 its center, σ_a the resonant cross section, σ_b the nonresonant cross section and q the line profile index.

This current experiment found E_0 , with no external field, to be in complete agreement with the earlier (1979) measurements by Hamm et al.²¹ The present data shows Γ to be 39 ± 2 meV in contrast to the previously measured value of 27.5 ± 0.8 meV. The values of both q and effective strength agree within experimental uncertainties. All of the fitted parameters are corrected for the 0.007 eV energy resolution of the experimental apparatus.

As the magnitude of the external field was increased, there was no observed shift in E_0 , until quenching occurred at a field strength of approximately 2.36 MV/cm. The effective strength of the resonant state appears to

decrease linearly with increasing field. The line shape index, q , is constant within statistical uncertainty, until the resonance disappears. There is, also, evidence that the resonance may narrow at fields below 1.25 MV/cm. It then broadens at higher fields before quenching.

The survival of the observed resonance in electric fields up to the 2 MV/cm indicate that it is of the "+" type similar to the shape resonance above $n=2$. There is a curious lack of evidence of mixing of adjacent angular momentum states as the field strength is increased. This may be due to the limit of the current experimental resolution.

Photodetachment cross section vs photon energy below the $n = 3$ threshold showing the two prominent dips.

Figure 1.5. Generalized QDT method theoretical fit(a) to the resonance below $n = 3$ data from Hamm et al.(b).²¹

Overview

As our experimental method is described, one should keep in mind what needs to be done to obtain the photo-detachment cross section.

1. Photo-excite the ion via a photon- H^- collision.
2. Determine the rate of production of H^0 , see equation 1.2.
3. Monitor the incident photon and ion fluxes.
4. Measure the wavelength (energy) of the incident photon.
5. Create an external electric field at the H^- -photon interaction region when needed.

The experimental apparatus used for this present investigation is essentially an updated version of the one used by Butterfield.²⁰ Details of the detector electronics and data acquisition methods are provided in chapter 3.

Doppler Tuning

The key to our ability to determine accurately the energy of the incident photon is the availability at LAMPF of the high quality, relativistic H^- ion beam, i.e. small angular divergence, narrow momentum spread and with particle velocities near the speed of light. The ions ride on the accelerating RF half cycle that cannot be used to accelerate protons. With these ultra-fast ions the relativistic Doppler shift can be exploited to produce a tunable photon source in the ion's rest frame.

For a given photon lab energy E_{lab} , the photon's energy in the H^- rest frame, is given by

$$E = E_{lab} \gamma (1 + \beta \cos \alpha). \quad (2.1)$$

$\beta = v/c$, where v = the speed of the ion in the lab frame, c = speed of light in a vacuum, $\gamma = (1 - \beta^2)^{-1/2}$, and α is the intersection angle of the photon and ion beams, such that $\alpha = 0$ is a head on collision. See Fig 2.2. For an ion beam with a kinetic energy of 650 MeV, a center of mass photon range of 1.523 eV to 14.25 eV can be obtained from a UV laser operating at wavelength of 266nm (4.65948 eV) in the lab. See Fig 2.1.

Our knowledge of the center of mass photon energy is based upon the how well we can determine the intersection angle, α , of the colliding beams and the velocity, β , of the ion beam. The photon energy resolution of the experiment has two components, the energy spread due to the angular uncertainty,

$$\delta E/E = \beta \gamma E_{lab} \sin \alpha \delta \alpha \quad (2.2)$$

and the energy spread due to the ion beam velocity,

Figure 2.1 Doppler tuning

An illustration of the dynamic range of doppler tuning at $\beta = 0.806$ for a lab photon energy of 4.65948.

$$\delta E/E = (\delta p/p) (\beta^2 + \beta \cos\alpha) / (1 + \beta \cos\alpha). \quad (2.3)$$

Note that if $\alpha = \cos^{-1}(-\beta)$ in eq. 2.3, the energy uncertainty due to the spread in the H^- beam momentum vanishes. This angle is called the "relativistic Doppler-free angle". For a 650 Mev ion beam this angle is approximately 144° .

Center of Mass Electric and Magnetic Fields

Motional barycentric electric fields in the megavolt per centimeter (MV/cm) range can be attained by further exploitation of our knowledge of special relativity. For a laboratory magnetic field, B' , perpendicular to the velocity of ion beam, v , an electric field orthogonal to both B' and v will exist with a field strength of

$$F = \gamma \beta c B'. \quad (2.4)$$

The center of mass magnetic field is

$$B = \gamma B'. \quad (2.5)$$

An ion beam with a β of 0.8062 (KE = 650 MeV) will see a transverse electric field of about 1 MV/cm and a magnetic

Figure 2.2 . Colliding H^- ion and photon beams.
 (a) Laboratory frame (b) Center of mass frame.

field of 5 kG from laboratory magnetic field of a modest 3 kG.

The analysis of data from the current experiment will ignore the influence of motional magnetic field on the ions. The ratio of the coupling energies is estimated by Bryant et al.¹⁹ and is

$$E_F/E_B = 2 \beta / \alpha, \quad (2.6)$$

where E_F is the coupling of the ion to the electric field and E_B is the coupling to the magnetic field. α is the fine structure constant (1/137). The ratio is about 200.

It is often desirable to excite pure substates of $M = 0$ or $M = \pm 1$. If the laser beam is polarized so that its electric field is parallel to center mass motional electric field (π polarization), the $M = 0$ state can be excited. Polarization perpendicular to the electric field (σ polarization) will excite the $M = \pm 1$ states.

Since the ion and photon beams will rarely be collinear, pure π polarization will not be achieved. Relativistic transformation from the lab to center of mass frame helps somewhat (for α less than $\pi/2$) through the aberration of light.⁶² The relativistic effect throws the light forward in the moving frame, i.e. α' is related to α by

$$\tan \alpha' = \sin \alpha / \gamma (\cos \alpha + \beta). \quad (2.7)$$

Calculating the Cross Section

The photodetachment cross section can be calculated using the relation²²

$$\sigma = \frac{(G R)(\beta \sin \alpha)}{[I J (1 + \beta \cos \alpha)]} , \quad (2.8)$$

where R is the rate of photodetachment fragment production, (see equation(1.2)). I and J are the photon and ion flux intensities. G is a geometric factor that represents the spatial and temporal overlap of the crossed beams. For two continuous, perfectly overlapping cylinders of the same radius r ,

$$G = (3\pi^2 rc)/16, \quad (2.9)$$

where c is the speed of light. This factor currently can only be estimated for the present experimental configuration and the cross sections presented here are therefore only relative.

Beam Parameters

Our photon source is a Quanta-Ray model DCR-2A Nd:YAG laser. In the Q-switched mode laser can be fired at a nominal rate of 10Hz. Maximum beam divergence is less than 0.5 milliradians. Its output is directed through a harmonic generator which can be configured to produce any one of three harmonics above its fundamental frequency. Table 3.1. lists the harmonics of the YAG.

Table 3.1 Output wavelengths of the Quanta-Ray YAG laser.

Harmonic	Wavelength (nm)	Photon Energy(eV) ⁶³
1 (fundamental)	1060	1.16487
2	532	2.32974
3	355	3.49461
4	266	4.65948

The linear accelerator at LAMPF can produce a pulsed H⁻ beam at a repetition rate of up to 120 pulses per second. The duration of each these macropulses is 500-700 microseconds. Each macropulse consists of 0.25 ns long micropulses spaced at 5ns, see Fig 3.1.

Figure 3.1 H^- beam pulse structure.

The ion beam's angular divergence is less than 1 milliradian. Its kinetic energy centroid has a FWHM of approximately 500 keV. The amount of radiation shielding in area B precludes the use of beam intensities higher than 100 nA. In practice, however, this experiment rarely sees beam currents exceeding 5 nA.

Beam Optics and Detectors

Our apparatus is located in experimental area B on the external proton beam (EPB or EP) line, see Fig 3.2 and 3.3. Ion beam focusing, up to the last three magnets in the beam path, is controlled by the accelerator operators in the central control room (CCR). The experimenters specify to the CCR personnel the required beam tuning, such as the spatial location of the beam with respect to the aperture of vertical bending magnet, SM02Y (see Fig 3.4). Adjustment of the current to SM02Y and the vertical bending magnets, VB1 and VB2, is under the direct control of the experimenters during the experiment. VB1 and VB2 are connected in series so that their magnetic fields are equal and in opposite directions. Thus a charged particle moving at a velocity v and deflected by an angle θ by VB1 will be deflected through an angle of $-\theta$ by VB2. CCR adjusts the beam so that it comes in below the nominal beam height at SM02Y.

Figure 3.2 LAMPF Plan View

Figure 3.3 LAMPF experimental areas

Figure 3.4 Photodetachment vertical bending magnets.

We, the experimenters, adjust the vertical benders and SM02Y to locate the beam in the scattering chamber, see below, to maximize its spatial overlap with the laser.

Sandwiching the interaction region are a pair of Helmholtz coils ("the Stark magnet") that provide the laboratory magnetic field at the photon- H^- collision point perpendicular the ion beam and, hence, crossed magnetic and electric fields in the center of mass. A pulse of current is sent through the coils which is timed to coincide with the photon pulse reaching the H^- interaction site. The timing of the current pulse is adjusted so that the magnetic field is constant before the beam pulses arrive and remains constant for a period much longer than the interaction photon-ion interaction. The magnet pulse duration is 1.8 μ sec and the laser pulse duration is 10 nsec. Details of the magnet development and operation are presented by Butterfield.^{20,64}

Any fragments of photodetachment will be either electrically neutral or positively charged. VB2 effectively separates H^0 and H^+ from the negative ion beam. The deflected particles are detected by placing a scintillation counter or fast ion chamber and Faraday cup in their respective paths. The particle trajectories are shown in Fig 3.4.

The YAG laser, mirrors and scattering chamber are mounted on an optical bench. The output of the laser/har-

monic generator is directed by the mirrors through a window at the bottom center of the evacuated scattering chamber and up to the mirrors of a turntable which is driven by a steel belt connected to a stepping motor. The angular position of the turntable, α , is digitized by an encoder attached to the turntable by another steel belt, as shown in Fig 3.5. The encoding scheme used here has an effective resolution of 18 bits per 2π radians, or about 31 microradians.

The laser has a beam diameter of approximately 6.5 mm. The H^- beam diameter is about 2mm. For the data presented in Chapter 4, a cylindrical lens was used to create a elliptically shaped photon beam cross section at the point of intersection with the ion beam, increasing the photon density in the interaction volume. See Fig. 3.6.

Laser beam intensity is sampled by vacuum photo-diodes and fast vacuum photodiodes positioned on the optical table to pick up scattered light from the mirrors in the beam line. A value for laser intensity at the interaction point is provided by a calorimeter inside of the laser beam catcher on the turntable in the scattering chamber.

Figure 3.5 The scattering chamber.

Figure 3.6 The cylindrical lens

Data Acquisition

It is helpful to examine the experimental procedure in general before describing the control electronics and function of the data acquisition system. Photodetachment spectra are obtained by

1. Rotating the turntable to establish the angle of intersection of the H⁻ and laser beams,
2. Measuring the number of photodetachment fragments (H⁰ and H⁺) for each laser "shot",
3. Continuing to measure at the selected angle until the accumulated charge collected by the Faraday cup from the H⁻ beam reaches a predetermined value,
4. Changing the angle of the laser beam by a fixed amount,
5. Going back to step 1 if needed.

A spectrum is generated by calculating the cross section at each angle and corresponding photon energy.

Let us define a run as the sequential measurement of cross sections at equally spaced preselected laser angle increments, usually less than 100 encoder steps. Data acquisition, turntable motor control, laser and magnet pulse timing are controlled by a PDP-11 minicomputer and other associated electronics. A block diagram of this

Figure 3.7 Block diagram of data acquisition configuration

system is shown in Fig 3.7. Just as the currents in the beam line magnets have to be adjusted to assure spatial overlap of the two beams. The control electronics must assure the temporal overlap of the laser pulse, an H^- micropulse, and the Stark magnet.

The laser intensity is high enough to present the possibility of having more than one photodetachment per laser pulse. This means that the number of photon- H^- interactions that occur during each laser "shot" needs to be determined. The pulses from the HO and H^+ scintillation detectors are counted, their amplitudes are digitized. A typical pulse height distribution is shown in Fig 3.8. The signals from the scintillators are gated and read only for the duration of the laser pulse. If more than one particle hits the detector while it is gated open, more energy is deposited, creating a larger pulse. Peaks for single, double, triple and more particle hits are clearly seen. If one assumes that the centers of the peaks are equally spaced, then one can define the slope, m , of the line as the inverse of the number of channels separating each peak. Therefore, the true number of photodetachments for a single value of photon energy will be the a sum of the laser shots scaled by the slope determined by the detector pulse height distribution. The low energy, i.e. low channel number, end of the spectrum may contain channels that represent no particles at all.

Figure 3.8 Real H⁰ pulse height distribution

A channel offset or pedestal(p_d) can be specified to eliminate counting the contents of those channels as events. For each angle (energy) sampled, the number times the laser actually fires, n_1 , is recorded, as is the integrated sum of the detector pulse height distribution, S_1 . The total number of particles to be used to calculate the number of photodetachment events is

$$\text{Total} = m (S_1 - n_1 p_d). \quad (3.1)$$

It should be emphasized that it is up to the experimenter to determine the slopes and pedestals for each detector and update the disk files used by the data acquisition software to calculate cross sections. The real time analysis does not calculate the slopes and pedestals from the height distributions.

The Q system acts as a director of user written program modules that control the experiment and associated electronics. It provides a standard set of commands to the user for starting and stopping a run, enabling or disabling data recording on magnetic tape and displaying histograms. Q also takes care of the details of loading machine code into the microprogrammable branch driver (MBD), the interface and data gateway between the experiment's electronics and the PDP11. Details of this realtime control environment are provided by the Q-Hand-

book65.

A number of editable text files, read by the routines controlled by Q, allow the experimenter to specify what data are to be read in and how they should be treated by the software. Experimental parameters such as the β of the H^- beam and lab energy of the laser can be quickly changed between runs. The slopes and pedestal values and histogram definitions are also easily modified without recompiling the set of Q programs that run the experiment.

Figure 3.9 is a schematic layout of the interface between Q, the experimental apparatus and the control electronics. The job of the electronic control during a run is threefold:

1. It has direct control of the electromechanical functions of the experimental apparatus. The firing of the laser must be timed so that the 5ns photon pulse arrives in the scattering chamber at the same time as the 0.25 ns bunch of H^- ions. The Stark magnet needs to be pulsed before every other laser shot. The details of the turntable stepping and angle encoder readout must be attended to.
2. It must collect and condition the analog

Figure 3.9 Control electronics

signals from the various photodiodes, particle detectors, and beam current monitors.

3. The computer must know the source and context of the data it is collecting whenever the Camac electronics is interrogated. An "event type" flag needs to be generated so that the computer knows what data to expect and what to do with it once it gets it.

Even though the experiment is computer controlled, it is driven by the physics of the current measurement. It is necessary for the experimenters to set up the electronics to insure that events of interest or, at least, potential interest, are collected.

Crucial to all of the above, is the knowledge of when a macropulse actually containing ions will arrive at the scattering chamber. The flash lamps of the laser must be triggered about 250 μ sec before the Q-switch to allow for optimum pumping. We are provided with a signal (LIOP) from the CCR computer which is generated only when a valid macropulse will arrive at the EPB. The signal timing with respect to the ions' real time of arrival can be adjusted to allow time for the laser to be pumped and Q-switch triggered.

The LIOP gate also controls the firing of the Stark magnet power supply. The magnet is pulsed before every other laser shot. Field on, field off, scattering events

are interleaved. This assures that other experimental variables are constant and changes in the photodetachment cross section are due solely to the applied external fields.

As stressed in Chapter 2, cross sections measured are relative, because of spatial and temporal uncertainties. The problem of synchronizing the arrival of the photons with a short burst of ions is exacerbated by the 5 ns output jitter of the laser. Typically the timing of the laser trigger is arranged so that a photon pulse occurs in the center of a macropulse.

The initial function of the NIM electronics, shown in Fig.3.9, at the start of an event, is to provide signals to the YAG laser and Stark magnet at the appropriate times.

If the laser actually flashes, a signal from a fast photodiode sampling the laser output is used to start data acquisition. If the laser, for any reason, does not fire nothing else will happen and no data will be taken. For each valid laser shot, the scintillation counters are read twice. The pulse heights gated in coincidence with laser are called "reals". Sixty μ sec after the laser shot, during the same macropulse, the detectors are read again and the results are called "accidentals". The "reals" signals contain information about any photodetachment fragments that have been produced plus any charged

particles that have been produced by gas stripping of the ions and other spurious particles. Assuming background conditions are constant over a 60 μ sec interval the "accidentals" will contain similar accidental counts to the ones folded into the laser related record. To obtain the actual rate of photodetachment, R from eq. 2.8 one need only subtract the accidentals from the reals,

$$R = \text{reals} - \text{accidentals.} \quad (3.2)$$

In the language of Q each different set of circumstances that generates data to be recorded is called an "event". The experimenter identifies each event with an event number. To make life simple, LAMPF has developed a Camac⁶⁶ module that allows each event to be identified by strobing a NIM logic pulse into a port corresponding to the event number. Hence, the computer software is able to identify event number via the information generated by the LAMPF trigger module.

It is the responsibility of the NIM electronics to time the generation of event trigger signals after all scalars and ADC's are ready to be read by the computer software.

Events used in this experiment and their functions are listed below:

Event 5 : Hardware and Software Clear

Clear all running sums required for histograms.
Clear all scalers, both NIM and Camac. Clear all ADC's. Read 32-channel ADC's, such as the laser catcher. Read the angle encoder.

Event 4 : End of Angle Event

Read and clear scalers that count number of laser shots. Read and clear Faraday cup scaler.

Event 8 : Update Scaler and Encoder Information

Read number of laser shots. Read number of Faraday cups. Read 32 channel ADC's, such as the laser catcher. Read the angle encoder.

Event 9 : Read after a Laser Shot with Stark Magnet Off

Read scintillation pulse height ADC's, both reals and accidentals. Read photodiode ADC's. Read fast ion chamber ADC's.

Event 10 : Read after a Laser Shot with Stark Magnet On

Functionally the same as Event 9, but all pulse heights and beam current readings are read by different ADC's and stored as different histograms. Both field and non-field cross sections are calculated simultaneously.

Introduction

Scaler and ADC information (encoder readings, photo-multiplier pulse heights, ion chamber outputs and photodiode signals) are written directly to 1/2" magnetic tape. Pulse heights from scintillation counters, laser intensity and instantaneous beam current are accumulated and can be displayed as histograms. The relative total scattering cross section (eq. 2.6) for each angle α (photon energy) is calculated and cross section versus incident photon energy can be displayed at any time during a run. A scan of 100 energy steps or less is taken. After a scan, the cross section information is printed on the line printer. These initial plots and print-outs, although useful for real time experiment diagnostics, require further analysis before definitive conclusions about experimental observations can be made. The location of $\alpha = 0$ as a function of encoder reading must be determined and an accurate value for the kinetic energy (hence β) of the H^- beam needs to be calculated before the energy location of features observed in the H^- photodetachment spectrum can be accurately calculated.

The experimental energy resolution, eq. 2.2 and 2.3, can be determined from the observed energy width of a feature in the H^- spectrum considered to be a δ -function for our purposes. For this current work the measured width of the $1p0$ Feshbach resonance, just below the

hydrogenic $n=2$ level was used. See Fig 4.1.

In some cases the counting statistics for the cross section measurement at each α are low. In these cases runs were rebinned using an energy increment approximately equal to the experimental energy resolution.

The Tools

Built into the Q data acquisition system on the PDP-11, is REPLAY. REPLAY simulates the actual experiment by replacing the CAMAC output to the PDP-11 with the raw data previously recorded on magnetic tape during the experiment. Before each run is REPLAYed experimental parameters such as the location of $\alpha = 0$, lab photon energy and H^- kinetic energy can be changed. ADC offsets (pedestals) and scaling factors (slopes) for cross section calculations can be modified.

One can, additionally, specify new bases for cross section normalization. For example, photodiodes are placed at various locations in the photon beam line to sample the intensity of the YAG laser. One might want to normalize the photodetachment cross section using the output of a photodiode that was read, but not used, for the cross section calculation during the actual experiment.

Figure 4.1 Gaussian fit to the Feshbach resonance
 This is an actual screen dump from the data analysis software. The Feshbach resonance sits on a sloping background which contributes to the asymmetric shape of the Gaussian curve.

Each run is given a number. Both Q and REPLAY produce two disk files. The files are identified by the run number with an extension of either ".DMP", a binary data dump or ".CRS", a text file, that is the image of the printout that is produced after each run. NCS, a program written by Butterfield,²⁰ can combine runs and/or recalculate the cross section for an energy step specified by the user.

After the cross sections are recalculated, it is useful to fit the features to a functional form. Since the PDP-11 in Los Alamos was not easily accessible to me, I chose to download the relevant ".CRS" files to be fit and analyzed to MS-DOS format floppy disks and perform all subsequent analysis on an IBM-PC.

A ".CRS" file consists of a header containing a list of the experimental parameters, ADC sum specifications (core histograms) and cross section normalization definitions (disk histograms as a function of core histograms). A table of the calculated cross sections as specified by the disk histogram definitions, as a function of energy, and angle follows.

The first member of the set of analysis tools for the IBM PC is CRSPARSE. It extracts two user specified columns of cross section values and their associated standard deviations. From the ".CRS" file CRSPARSE creates ".FIT"

and an ".DTA" file that can be read and manipulated by subsequent curve fitting and plotting programs.

The data is fit to a Fano line shape, discussed below, by a program that performs a nonlinear least squares fit to a user supplied, arbitrary functional form. I made substantial modifications to an existing program so it would calculate the standard deviations of fitted parameters, read and write files compatible with other programs used for data analysis. An external, editable parameter file allows the user to specify initial values for free parameters to be fitted. A corresponding flag can be set for each parameter and force it to maintain its initial value.

Because the cross sections measured in this experiment are relative, a program had to be written to normalize the cross section values so that they could be compared in a straightforward way.

Graphical presentation of data is almost a necessity. I created a plotting program to display the experimental cross sections, standard deviations (as error bars), and the fitted function on one graph. All of the plots in this chapter were generated with this program.

Listings appear in the appendix. The data analysis process is summarized in Fig 4.2.

Calculations such as conversions between lab photon energy and encoder angle, determination of the H^- beam

energy, predictions of the encoder settings of features in the H^- spectrum, and tabulation of fitting analysis summaries were easily performed and displayed using a spreadsheet program on the "PC"⁶⁷. These spreadsheet templates also proved useful during the experimental runs, when quick analysis was needed to interpret incoming spectra.

Fitting the Data

Fitting of the experimental data was done in three phases.

1. Calibration of the data to a feature in the H^- spectrum whose energy is known.
2. Normalization of the measured relative cross sections to a consistent value.
3. Fit the normalized spectra to a functional form.

The $1p^0$ Feshbach resonance below $n=2$ was used as an energy benchmark. Its location has been well established in previous experiments⁶⁸, and the feature is easily accessible for measurement. It can be measured with the same experimental configuration as the resonances of interest in this work near the hydrogenic $n=3$ level. With a ion beam kinetic energy of 650 MeV, the Feshbach is located about 10^0 away from the $n=3$ region. Calibration runs near $n=2$ are interspersed in the $n=3$ runs, assuring

Figure 4.2 Block diagram of fitting procedure

similar observational conditions. The location of the Feshbach splitting with increasing external electric fields, tracking the Stark shift of $n=2$ level,¹⁹ providing a cross check for the Stark magnet field values.

Since α for the Feshbach resonance should be the same on both sides of the ion beam, the resonance is also used to determine the encoder reading for which $\alpha = 0$. Finding $\alpha = 0$, is a pure geometric exercise. Once it is known, the value of β can be adjusted to place the resonance at the correct absolute angle location, eq 2.1.

The values we obtain for the photon- H^- cross section are reliable up to a geometric factor, G , eq 2.8. It can be safely assumed that during one run, lasting about one hour, conditions are usually constant. The relative photodetachment cross sections measured during a run will be internally consistent. Over the course of a day or two, beam intensities and positions of both ion and photon beam will change sufficiently to yield different relative cross sections at the same energy. I have chosen to normalize all cross sections so that the cross section furthest from and lowest in energy from the resonance has the same average value. The weighted average of the five lowest energy points of a scan with no external electric field is used as to compute a normalization factor for both field and no field data. I define the weighted average $\langle B \rangle$ as,

$$\langle B \rangle = (\Sigma B_i / \sigma_i^2) / (\Sigma 1 / \sigma_i^2) \quad (4.1)$$

where B_i is the i th data value and σ_i is its associated standard deviation. The average of the standard deviation $\langle \sigma \rangle$ can be found by taking the inverse of the sum of the reciprocals of the squares of the individual σ_i 's, that is

$$1/\langle \sigma^2 \rangle = \Sigma 1/\sigma_i^2. \quad (4.2)$$

The observed cross sections near $n=3$ have been fitted to a Fano line shape introduced by Fano and Cooper⁶⁹ and used by Hamm et al.²¹ in their analysis of the field free shape of this $1p^0$ resonance. The functional form which arises from the coherent addition of the amplitude of a Breit-Wigner⁷⁰ resonance and constant continuum is

$$\sigma(\epsilon) = \sigma_a \frac{(q + \epsilon)^2}{1 + \epsilon^2} + \sigma_b, \quad (4.3)$$

where $\epsilon = (E - E_0)/(\Gamma/2)$, with Γ being the FWHM of the resonance, E_0 its center, σ_a the resonant cross section, σ_b the non resonant cross section and q the line profile index.

Fano³⁰ has pointed out that it is probably not

physically reasonable to assume that the width parameter, Γ , is constant with respect to energy in the region of a resonance. Early in the development of the fitting programs for the analysis of the current data, I experimented with spectral shapes that contained a Γ that varies linearly with energy, (more precisely $E - E_0$). In place of the Fano line shape, I used the Breit-Wigner line shape described by,

$$\sigma(E) = \sigma_a \frac{(\Gamma/2)^2}{(E-E_0)^2 + (\Gamma/2)^2} + \sigma_b. \quad (4.4)$$

I made Γ , normally assumed to be a constant, a function of $(E-E_0)$, that is $\Gamma(E-E_0) = \alpha + \beta(E-E_0)$, where α and β are constants.

For the appropriate choice of α and β , the line shape obtained fits a Fano shape to an arbitrary numerical precision. Chi-squared for the fit was less than 0.001 for 50 degrees of freedom. The problem with the function is that the value of E_0 is shifted with respect to the Fano value. A modified Breit-Wigner shape function was fit to a Fano form. The fit, illustrated in Fig. 4.4 with parameters listed in Table 4.1, was exact. At this time there is no strong theoretical justification for discarding the Fano line shape in favor of another way of parameterizing the same function. I have, therefore, chosen to use Fano functional form.

Table 4.1 Corresponding Breit-Wigner and Fano parameters

=====

Fano parameters:

E_0	12.650
Γ	0.045
q	-0.684
σ_a	3.970
σ_b	5.046

Breit-Wigner parameters:

E_0	12.617
α	0.141
β	2.928
σ_a	5.845
σ_b	5.030

Figure 4.3 Comparison of Breit-Wigner to Fano line shape. Parameters for these two curves are listed in Table 4.1. The two curves lie on top of one another.

As further check on the validity of the fitting algorithm used, I generated twenty sets of Monte-Carlo data from a "parent" Fano function, fitted the data, then took the weighted average of the resulting parameters to compare with the "parent" parameters. Monte Carlo data points were generated by calculating the value of the Fano function at a chosen energy then shifting it using a Gaussian random offset of a standard deviation comparable to the actual data. The statistical error, depicted by error bars in the figures below were calculated in the same way. Table 4.2 compares the "parent" parameters to the fits to Monte Carlo data. Comparing these data with those in Tables 5.1 and 5.3, it is clear that the central value of the fitted parameters as well as their errors are comparable. Figure 4.4 shows two typical data sets.

Table 4.2 Parameters of Monte Carlo data fits compared to "parent" Fano function.

Parameter	"parent"	weighted average of fits
=====		
E_0	12.650	12.650 ± 0.001
Γ	0.045	0.042 ± 0.002
q	-0.684	-0.655 ± 0.04
σ_a	3.970	3.967 ± 0.2
σ_b	5.047	5.060 ± 0.2

Figure 4.4 Sample plots of Monte Carlo data.
Note that this is NOT real experimental data.

Energy Resolution

Figure 4.1 shows a Gaussian fit to the Feshbach resonance below $n=2$. A number of "Feshbach" runs were fit using both the PDP-11 minicomputer in Los Alamos with software provided by LAMPF and my own fitting programs on the PC. Assuming that the Feshbach resonance is infinitesimally wide, one must conclude that the observed width is due solely to the energy resolution of our experimental apparatus. The fits to the Fano line shape must be corrected for experimental resolution. The real value of each data point is distributed over a finite resolution width. This spreading or "smearing" can be simulated by the convolution of the assumed functional form of the energy spectrum with a Gaussian resolution function. The value obtained by measurement of the total cross section at the point E is really

$$f(E) = \int f(E') A \exp[-(E-E')^2/2\sigma^2] dE'. \quad (4.5)$$

It is a straightforward matter to write a computer program to perform this numerical integration in the neighborhood of each data point. A systematic study was made examining the effect of a Gaussian resolution function on the Fano line shape to obtain a reasonable estimate of the effect of smearing on our observations.

A Fano form was chosen whose parameters q , E_0 , Γ , σ_a and σ_b were typical for this present experiment. I wrote a

computer program to create a set of smeared data points. The energy resolution and the limits of integration could be adjusted by editing a parameter file on disk. The resulting set of data was fitted to the Fano line shape as if it were real experimental data and the results were compared to the values of the function before smearing.

Of all of the parameters only Γ , the width, is sensitive to small changes in resolution. The remaining parameters are effected only when the resolution exceeds the value of Γ . This illustrates how electron scattering experiments can detect features in a spectrum whose widths are on the order of experimental resolution. Figure 4.4 shows the effect of decreasing resolution on the measured value of Γ . Note that for values of experimental resolution that are less than $\Gamma/2$, the resolution adds quadratically with the true Γ .

For our assumed energy resolution of 7 meV, one need only adjust the Γ . This can be done by subtracting the 7 meV in quadrature i.e.

$$\Gamma_{\text{true}} = (\Gamma_{\text{obs}}^2 - (0.007)^2)^{1/2}. \quad (4.6)$$

A graphical summary of the effect of energy resolution upon effective strength is illustrated in Figure 4.6. Note that for this experiment's resolution of 7 meV, a reliable measurement of effective resonance strength is obtained.

Figure 4.5 Width vs experimental resolution (line A) Width added to resolution in quadrature. (line B). The experimental resolution for this investigation of 7 meV was deduced from a Gaussian fit to the Feshbach resonance near $n=2$.

Figure 4.6 Effective strength vs energy resolution.

The results of the analysis for scans in the energy region of the $1p_0$ resonance are presented here. As detailed in chapter 4, each set of data was fit to a Fano line shape. For each fitting calculation E_0 , Γ (the width), q , σ_a and σ_b were free parameters. Both the parameter values and standard deviations were calculated.

The fitting algorithm used is a rigorous least squares adjustments based upon a method outlined by Wentworth⁷¹ and Demming⁷². In order to correct for the energy resolution of the experimental apparatus, the resolution was subtracted in quadrature from the fitted value of the width(Γ). The results of the resolution study described in the last chapter indicated that other fitted Fano parameters were not significantly sensitive to resolutions of 20 meV or less; no corrections were calculated.

To evaluate the response of the resonance to an external electric field, the effective strength of the resonance is also computed⁷³.

$$E.S. = (\sigma_a / (\sigma_a + \sigma_b))^2 (q^2 + 1) \quad (5.1)$$

The effective strength of the resonance near $n=3$, with no-field is 0.34, compared to the value of the shape resonance of about 35.¹⁹ This two order of magnitude difference in effective strength makes the $n=3$ resonance much more difficult to measure since it is a much less prominent a feature in the H^- continuum.

The Resonance with No External Field

It is instructive to examine first the spectra obtained with no external electric field. These can be compared to earlier experimental results.²¹ Since "no-field" scans come with every run taken (see chapter 3) a substantial amount of data was generated. Tables 5.1 and 5.2 present fitted parameters and calculated values of all of the scans taken in the energy region of the $1p_0$ resonance with different an external electric field. Seven typical data sets and their corresponding fits are shown in fig 5.1.

The scans in this series, Figure 5.1c,d and f that extend through 12.83 eV, the measured location of the second recursion of the $1p_0$ resonance. This scan provides no conclusive evidence for the second "dip".

Table 5.3 compares the corrected no-field weighted average of this work with the results of Hamm et al.. The superimposed line shapes generated from the fitted parameters of the Hamm data and the no-field values from this current investigation are shown in Fig. 5.2. There is a disagreement in Γ for the two experiments. The researchers in the former experiment did not have access to as well defined energy scale as this present experiment. Cross section data from different runs were arbitrarily shifted in energy so that data points visually lined up; this could have contributed to the significant

significant difference in the value of width parameter since this is the most sensitive to small changes in energy.

Table 5.1 and 5.2 Summary of normalized runs.

Explanation of Table Headings

E(MV/cm) : The value of the center of mass external electric field.

std dev : Statistical uncertainty (listed directly below the fitted or calculated value).

offset : The energy difference in eV from 12.650 eV.

con level : The confidence level of the fit.

eff strth : The effective strength, see eq 5.1.

CVR : Voltage across the shunt resistor in the Stark magnet power supply.

The laboratory B-field = $960 \times \text{CVR}$.

Table 5.1 Fitted parameters of energy scans

run# E(MV/cm)	EO std dev	Width	q	sigm_a	sigma_b
=====	=====	=====	=====	=====	=====
no_fld_avg 0.0	12.6500 0.0010	0.0390 0.0020	-0.7169 0.0372	4.1054 0.2000	4.4770 0.1350
5278mzn 1.18	12.6502 0.0052	0.0581 0.0081	-0.5807 0.1211	2.7747 0.4138	6.5317 0.2884
5279mzn 2.36	12.6203 0.0100	0.0568 0.0221	-3.0960 1.5006	0.1907 0.1880	9.3402 0.1680
5280mzn 2.36	12.6206 0.0266	0.1118 0.0377	-1.3369 0.8607	0.5060 0.8167	7.8701 0.2100
5281mzn 0.69	12.6463 0.0032	0.0357 0.0059	-0.9809 0.1782	2.3206 0.5102	4.9730 0.3074
53712mzn 0.24	12.6457 0.0023	0.0323 0.0054	-0.7842 0.1032	4.6676 0.6601	5.9586 0.5694
5291mzn 2.36	12.5887 0.0284	0.0905 0.0416	-1.9103 0.9750	0.4724 0.7862	8.6113 0.3357
5374dmzn 0.79	12.6328 0.0041	0.0444 0.0082	-0.9231 0.1410	3.5910 0.6480	5.0871 0.5058
5375dmzn 1.18	12.6365 0.0046	0.0191 0.0095	-0.6505 0.2428	3.2362 1.2949	5.7002 1.2365
5377mzn 1.97	12.6455 0.0162	0.0854 0.0480	-0.4620 0.2116	2.2562 0.7020	6.0556 0.5770

Table 5.2 Calculated parameters for energy scans

run#	CVR E_fld(MV/cm)	chi_sqd #of pts	offset con lev	eff_strth std dev
=====				
no_fld_avg	0.00	--	0.0000	0.35
	0.00	--	--	0.022
5278mzn	3.00	34.04	0.0002	0.12
	1.18	41.00	0.56	0.028
5279mzn	6.00	33.69	-0.0297	0.004
	2.36	42.00	0.62	0.009
5280mzn	6.00	22.88	-0.0294	0.01
	2.36	38.00	0.91	0.03
5281mzn	1.50	41.33	-0.0037	0.19
	0.69	34.00	0.067	0.07
53712mzn	0.60	18.39	-0.0043	0.31
	0.24	27.00	0.68	0.06
5291mzn	6.00	41.76	-0.0613	0.01
	2.36	40.00	0.21	0.041
5374dmzn	2.00	44.04	-0.0172	0.31
	0.79	45.00	0.31	0.081
5375dmzn	3.00	29.56	-0.0135	0.18
	1.18	48.00	0.94	0.11
5377mzn	5.00	85.27	-0.0045	0.09
	1.97	79.00	0.19	0.043

Figure 5.1 Typical no-field spectra

Figure 5.1 Typical no-field spectra (cont'd)

Table 5.3 Comparison of corrected fitted parameters for a fit. (The weighted average of all no field scans) to Hamm et al..

Parameter	Hamm et al.	This experiment
E_0	12.650 ± 0.004	12.650 ± 0.001
Γ	0.0275 ± 0.0008	0.0390 ± 0.002
q	-0.81 ± 0.02	-0.716 ± 0.37
σ_a	--	4.11 ± 0.200
σ_b	--	4.47 ± 0.135
effective strength	0.32 ± 0.02	0.34 ± 0.02

Figure 5.2 Comparison of line shape from Hamm et al.21 and the no-field data from the present work. The line with the small squares is the Hamm data.

Effects of the External Field

Figure 5.3 represents measurements taken within in a few minutes of each other, and shows very well the progression of the shape of the $1p_0$ as the applied external electric field is increased. An illustration of the complete quenching of the $1p_0$ resonance in a strong (2.36 MV/cm) external electric field is run 5280 shown in Fig. 5.3d.

The spectra in Fig. 5.3 provide a qualitative feel for the effect of the increasing electric field on the resonance. By examining the effect of the field on each fitted Fano parameter more quantitative knowledge about the behavior of the resonance can be gained. Resonance quenching is illustrated in Figure 5.4d, which shows the effective strength as a function of external field. The data have been fit to a straight line. Although the electric field intercept of the linear fit is 2.6 MV/cm, this is too high a value to be considered the field required for full quenching. Fits using the highest field data cannot be relied upon to give consistent results. Comparing a number of scans taken at 2.36 MV/cm in Fig. 5.5, one is forced to conclude that the resonance has been completely quenched.

Figure 5.4c indicates no definitive shift in E_0 as the external field is increased. As pointed out above, it is

Figure 5.3 Comparison of the shape of the $1p_0$ resonance in increasing external electric fields. The Fields are (a) no field, (b) 0.69 MV/cm, (c) 1.18 MV/cm, (d) 2.36 MV/cm.

safe to disregard the data points at the highest field values.

A study of the width(Γ) data in Fig 5.4b reveals what appears to be a plateau in value of Γ , below the electric field values of 1 MV/cm. A similar tendency for the resonance to narrow before broadening has also been identified in the behavior of the shape resonance just above $n=2.74$

Figure 5.4 Summary of electric field strength vs fitted parameters.

(a) $-q$, (b) Γ , (c) E_0 , (d) Effective strength.

The last set of plots, Fig. 5.6, in this chapter presents a graphical summary of the parameters obtained by fitting a selection of no-field scans. The ordinate for each of the charts is an arbitrary run number, chosen so that the data points are evenly spaced vertically. Each datum is displayed as a central value plus a horizontal "error bar" indicating the standard deviation for the fit.

As a guide to the reader in judging the consistency of the fits, a superposition of a Gaussian probability function for each parameter has been calculated. The area of the Gaussian for each fitted parameter is $1/\sigma$. Using a weight of $1/\sigma$ instead of $1/\sigma^2$, as one does to compute a weighted average, tends to emphasize systematic errors over statistical ones.⁷⁵ For totally consistent experimental data the resulting plot, an ideogram, should be a symmetric curve with a single peak. An ideogram is superimposed on each graph in Figure 5.5. The weighted averages of these parameters are tabulated in Table 5.3 and displayed as a vertical line plotted at the appropriate location on each chart in Figure 5.5.

It must be noted that the paucity of scans is due to a great extent to a catastrophic failure of the accelerator system itself during the second phase of this experiment. Ion beam conditions that will allow further study of this resonance will not be available for at least two years. As the reader has seen, the present analysis of the small

amount of existing data showing the behavior of the $1p_0$ resonance in an external field allows valuable conclusions to be drawn.

Figure 5.5 The 1p₀ resonance fully quenched

Figure 5.6 Summary of no-field parameters
(a) E_0 , (b) $-\Gamma$, (c) Γ

Figure 5.6 Summary of no-field parameters (cont'd)
 (d) Effective strength, (e) σ_a , (f) σ_b

The experimental technique used here is sophisticated and elegant and has been, in many instances, the sole source of empirical information by which theoretical investigators can check the validity of their work.

Using the photon as a probe to investigate correlated motion of atomic electrons is not without its limitations. Although our technique has an extremely high signal to noise ratio when compared to plasma or electron collision experiments, count rates are often low. Single photon excitation, from the ground state, provides access to only one angular momentum state. (Compare the spectrum of Williams Fig 1.4 to Hamm et al. Fig 1.6).

The work documented in the previous chapters is the first systematic study of the response of the $1p^0$ resonance at $n=3$ to external electric fields. Measurement of the resonance spectrum near the $n=3$ threshold presents a greater experimental challenge than the region near $n=2$, since the effective strength of the $n=2$ shape resonance (35) is approximately 100 times that of the $1p^0$ resonance at $n=3$ (0.34).

The present investigation clearly shows the quenching of the resonance as a function of external field strength. Substructure is not evident. There was no evidence mixing of nearby states, i.e. S and D states, with the P state. The resistance to quenching in external fields less than 1.5 MV/cm supports the putative "+" classification of the

observed state. The "+" state, shape resonance, just above $n=2$ exhibits the same durability in strong electric fields.

It is interesting to compare the hyperspherical potentials at $n=3$ to the ones calculated for the resonances near $n=2$ by Lin (see Fig. 1.3). Lin⁵ points out that as the external field increases, the potential well gets narrower. At sufficiently large fields the well can no longer support a bound state. As increasing electric fields narrows the potential barrier, the lifetime of the resonant state decreases through quantum mechanical tunneling.

One would expect a downward shift of E_0 , tracking the downward quadratic Stark shift of the $n=3$ hydrogenic threshold itself as greater values of electric field are applied.⁷⁶ The statistical uncertainty exhibited in data sets such as Fig. 5.4c would tend to obscure any detectable shift in E_0 .

A lack of noticeable change in E_0 could be due to the Stark shift and potential narrowing working against each other. One would expect E_0 to rise as the potential well narrows, thus cancelling the downward Stark shift.

There is a possibility that the line shape narrows at moderate fields. A detailed study at moderate fields would provide more substantial evidence to confirm or deny the existence of this narrowing. Understanding the mechanism

of the narrowing, possibly due to coherent mixing with narrower resonances, could also shed light on the mechanism of quenching itself. Measurements performed with light of a known polarization exhibit very low counting statistics. For example run number 5375 in Fig. 5.1e does not allow us to make conclusions about the behavior of "M" states in electric fields using vertically polarized photons.

There is lack of agreement of the fitted width (Γ) of the present no-field data and that of the only previous measurements.²¹ Energy calibration and the validity of fitting routines used in this investigation have been carefully verified, see chapter 4. Hamm et al. combined cross sections and shifted their energies from multiple runs before fitting the data.²¹ This may have caused a distortion of the shape of the fit, effecting the most sensitive parameter, Γ , most noticeably. The disagreement will need to be resolved by gathering further experimental data in the future.

Hamm et al.²¹ reported a second recursion of the 1p σ resonance at about 12.83 eV, is not evident in this study. Its existence, in this work, may be masked by the high statistical error of the scans that covered this region.

To summarize the findings of this investigation one can say the following:

1. The width of the n=3 resonance, in external

electric fields below 1MV/cm, remains relatively constant, before broadening at higher field values. A similar phenomenon has been observed in the shape resonance just above $n=2$.

2. A downward shift of E_0 with increasing external field strengths has not been conclusively observed.

3. The $1p_0$ resonance quenches completely at a field strength of greater than 2.36 MV/cm.

Within our present experimental resolution the location of the $1p_0$ resonance has been reconfirmed. Its quenching in a strong external electric field has been, for the first time, documented. Its behavior in moderate fields has been shown.

Appendix 1. Listing of Gaussian Smearing Generator.

```

program smeardta;
(
  Reads prefix from the command line along with the number of iterations
  to be done by fitting program.
  Uses the extension .TLP for the CRS file. This can be changed by
  changing the constant tlp below.
  - Stan Cohen

```

Revision History;

```

    06/20/85  added getweight function -SC
    06/20/85  disabled show data         -SC
    06/22/85  changed tlp def to .crs read from a crs file -SC
    06/24/85  corrected bug in parsing to last column -SC
    07/22/85  include sigma b in fit file list
    07/23/85  read FIT.PAR for fit parameters
    07/23/85  reads a dta file and makes a fit file
    07/30/85  reads new HOLDFIT.PAR and convergence criterion
    08/12/85  modified x-y dump routine and list_points

```

Read in Fano parameters of a fitted run then smear points by
convoluting with a gaussian energy resolution of given
(read in) FWHM.

- Stan Cohen 28 Oct 1985

```

}
const
  maxnums = 300;
  maxpars = 4;
  comma = ',';
  blank = ' ';
  semi_c = ';';
  dot = '.';
  nulstr = '';
  dta = '.dta';
  crs = '.crs';
  fit = '.fit';
  FWHMtoSigma = 0.42481;
  sqrttwoPI = 2.506628;
type
  str20 = string[20];
  str35 = string[35];
  str80 = string[80];
  rearray = array [1..maxnums] of real
var
  fname : str20;
  xaray, yaray, sigmx, sigmy : rearray;
  arraycnt, headcnt, xcolumn, ycolumn, l : integer;
  the_file : text;
  fitparm : array[1..maxpars, 1..2] of str35;
  E0, q, gamma, sigma_a, sigma_b, res, deltaE : real;
  grid_size : integer;
  xlabel, ylabel : str20;
{-----}
function newfilename : str20;
var

```

begin

newfilename := ParamStr(1);

end;

{-----}

procedure getxandy(var actcnt: integer);

var

i : integer;

thename, trash : str20;

mydata : text;

begin

thename :=concat(fname,dta);

writeln('Reading in : ',thename);

write('Reading .');

assign(mydata,thename);

reset(mydata);

actcnt := 0;

readln(mydata, xlabel);

readln(mydata, ylabel);

while not eof(mydata) do

begin

actcnt := actcnt + 1;

if (actcnt mod 10 = 0) then write('.');

read(mydata,xaray[actcnt]);

readln(mydata,sigmx[actcnt]);

read(mydata,yaray[actcnt]);

readln(mydata,sigmy[actcnt]);

end;

close(mydata);

writeln;

end;

{-----}

function Gauss (a_sqd, Gsig : real) : real;

begin

Gauss := exp(-a_sqd / 2.0) / (sqrttwoPI * Gsig)

end;

{-----}

function Fano (the_E, Ez, gam, the_q, siga, sigb :real) :real;

var

epsi : real;

begin

epsi := 2.0 * (the_E - Ez) / gam;

Fano := sigb + siga * sqr(the_q + epsi)/(1.0 + sqr(epsi))

end;

{-----}

function smear (Ei, del_E, resol : real;

steps : integer) : real;

var

Eoff, estep, Zoffsq, sigma_s, rsteps : real;

fano_part, gauss_part, temp_smear : real;

offcnt, k :integer;

```

begin
  temp_smeas := 0.0;
  rsteps := steps; { fix integer to real }
  sigma_s := resol * FWHMToSigma;

  if steps >= 1 then
    estep := del_E / (rsteps - 1)
  else
    estep := sigma_s * sqrttwoPI;

  { Simpson's rule for numerical integration }

  k := 1 + (steps div 2);
  for offcnt := 1 to steps do
    begin
      Eoff := Ei - (offcnt - k) * estep;
      Zoffsq := sqr((Eoff-Ei)/sigma_s);

      fano_part := Fano(Eoff,E0,gamma,q,sigma_a,sigma_b);
      gauss_part := Gauss(Zoffsq, sigma_s);
      temp_smeas := temp_smeas + fano_part * gauss_part
                      * estep;

    end;
  smear := temp_smeas;
end;
{-----}
function readint(promptvar:str20):integer;
var
  tempint : integer;

begin
  {This has been modified to read from the disk file smear.par
   see getparms }
  { write('Enter ',promptvar,' = ');}
  readln(the_file,tempint);
  readint := tempint;
end;
{-----}
function readreal(promptvar:str20):real;
var
  tempreal : real;

begin
  {This has been modified to read from the disk file smear.par
   see getparms }
  { write('Enter ',promptvar,' = ');}
  readln(the_file,tempreal);
  readreal := tempreal;
end;
{-----}
procedure getparms;
begin

```



```

{read in global vars
  modify readreal & readint if you want to read from
  the console. once again -SC }
assign(the_file,'smear.par');
reset(the_file);
grid_size := readint('grid_size');
E0 := readreal('E0');
q := readreal('q');
gamma := readreal('gamma');
sigma_a := readreal('sigma_a');
sigma_b := readreal('sigma_b');
deltaE := readreal('deltaE');
res := readreal('resolution');
close(the_file);
end;

{-----}
procedure smearpoints(npts : integer);
var
  i : integer;
begin
  write('Smearing. ');
  for i := 1 to npts do
    begin
      if (i mod 10) = 0 then write(dot);
      yaray[i] := smear(xaray[i],deltaE,res,grid_size);
    end;
  writeln
end;

{-----}
procedure get_pars;
const
  parfile = 'FIT.PAR';
var
  i : integer;
  pardata : text;
begin
  assign(pardata,parfile);
  reset(pardata);
  for i:= 1 to maxpars do
    begin
      readln(pardata, fitparm[i,1]);
      readln(pardata, fitparm[i,2]);
    end;
  close(pardata);
end;

{-----}
procedure list_pts (ttlpts : integer);
const
  maxpars = 4;
  comma = ',';
  one = 1.0000;

```

```

var
  pind, coord, dummy, parent, i : integer;
  varfile : text;
  fitname : str20;

begin
  fitname := concat(fname, fit);
  writeln('Saving to : ', fitname);
  get_pars;
  assign(varfile, 'fitfile.dat');
  rewrite(varfile);
  writeln(varfile, fname);
  close(varfile);
  assign(varfile, fitname);
  rewrite(varfile);
  writeln(varfile, tlpts);
  writeln(varfile, ParamStr(2), comma, fitpara[1,2]);
  writeln(varfile, '1,0');
  writeln(varfile, '0.5');
  write('Saving .');
  for coord := 1 to tlpts do
    begin
      if (coord mod 10) = 0 then write(dot);
      write(varfile, yarray[coord], comma, one, comma);
      writeln(varfile, xarray[coord], comma, one);
    end;
    for parent := 2 to maxpars do
      writeln(varfile, fitpara[parent,1], comma, fitpara[parent,2]);
    writeln(varfile, 'SigA, ', sigma_a, ', 0');
    writeln(varfile, 'SigB, ', sigma_b, ', 0');
    close(varfile);
    writeln;
  end;
  {-----}
  {----- main loop control -----}
  procedure maincontrol;
  begin
    fname := newfilename;
    getparams;
    getxandy(arraycnt);
    smearpoints(arraycnt);
    list_pts(arraycnt);
  end;
  {----- checkfor all params -----}
  begin
    if ParamCount = 2 then
      maincontrol
    else
      (Abort)
    writeln ('Usage: [file prefix] [number of fit iterations]');
  end.{ smeardata }

```

Appendix 2. Listing of CRS File Parsing Program

```

program crsparse;
{
    CRS file parser
    Reads prefix from the command line along with the number of iterations
    to be done by fitting program.
    Uses the extension .TLP for the CRS file. This can be changed by
    changing the constant tlp below.
    - Stan Cohen
}

Revision History;
    06/20/85    added getweight function -SC
    06/20/85    disabled show data      -SC
    06/22/85    changed tlp def to .crs read from a crs file -SC
    06/24/85    corrected bug in parsing to last column -SC
    07/22/85    include sigma b in fit file list
    07/23/85    read FIT.PAR for fit parameters
    08/12/85    changed lst_point to make file to be read by
                ffithold.exe
}

const
    maxmess = 2;
    maxnums = 300;
    maxheads = 20;
    maxlen = 132;
    E = 'E';
    minus = '-';
    blank = ' ';
    semi_c = ';';
    dot = '.';
    nulstr = '';
    angle = 'ANGLE ';
    data = 'DATA';
    dta = '.dta';
    tlp = '.crs';
    fit = '.fit';

type
    str20 = string[20];
    str35 = string[35];
    str80 = string[80];
    str132 = string[132];
    messages = array[1..maxmess] of str80;
    numarray = array [1..maxnums] of str35;
    headarray = array [1..maxheads] of str35;
var
    header : str132;
    fname : str20;
    dataflag : boolean;
    headings : headarray;
    xaray, yaray, sigmx, sigmy : numarray;
    errmess : messages;
    arraycnt, headcnt, xcolumn, ycolumn, l : integer;
    the_file : text;
{-----}

```

```

function yesorno (prompt : str80):boolean;
var
    nfn : str20;

begin
    yesorno := false;
    write(prompt);
    readln(nfn);
    if (nfn = 'Y') or (nfn = 'y') then yesorno := true;
end;
{-----}

function newfilename :str20;
var
    nfn : str20;

begin
    newfilename := ParamStr(1);
end;
{-----}

procedure open_the_file (var mydata : text);
var
    thename : str20;
begin
    thename := concat(fname, tlp);
    assign(mydata, thename);
    reset(mydata);
end;
{-----}

function go_to_head (var mydata : text ;
    var headrow : str132;
    keyword : str80 ) : boolean;
var
    fname, firstchars : str80;
    keylen : integer;
    gotit : boolean;
begin

    keylen := length(keyword);
    gotit := false;
    go_to_head := true;

    repeat
        if eof(mydata) then
            begin
                gotit := true;
                go_to_head := false;
                headrow := ''; {Null string}
            end
        else
            begin

```

```

    readln(mydata, headrow);
    firstchars := copy(headrow, 1, keylen);
    if (firstchars = keyword) then
        gotit := true;
    end;
until gotit;
end;
(-----)
function eatblanks (mystring : str132;
    var startat : integer) : boolean;
var
    inlen : integer;
    noomore : boolean;
begin
    inlen := length(mystring);
    startat := startat - 1;
    repeat
        startat := startat + 1;
        noomore := (startat = inlen);
    until (blank () copy(mystring, startat, 1)) or noomore;
    eatblanks := noomore;
end;
(-----)
function eatchars (mystring : str132;
    var startat : integer) : boolean;
const
    maxlen = 132;
var
    inlen, minus_count : integer;
    currchar : char;
    noomore, isblank, eflag : boolean;
begin
    minus_count := 0;
    eflag := false;
    inlen := length(mystring);
    startat := startat - 1;
    repeat
        startat := startat + 1;
        noomore := (startat = inlen);
        currchar := copy(mystring, startat, 1);
        isblank := (blank = currchar);
        if currchar = E then eflag := true;
        if eflag and (currchar = minus) then
            begin
                minus_count := minus_count + 1;
                if minus_count = 2 then
                    begin
                        isblank := true;
                        (startat := startat - 2);
                    end;
                end;
            end;
        until isblank or noomore;
    eatchars := noomore;

```

```

end;
{-----}
procedure check_tail( var the_string : str35);
var
    the_len : integer;
begin
    the_len := length(the_string);
    if minus = copy(the_string,the_len,1) then
        the_string := copy(the_string,1,the_len -1);
    end;

{-----}
function get_nth_item (input_str : str132;
    var theitem : str35;
    var item : integer) : boolean;
var
    cntr, charcntr, index : integer;
    out_of_chars, out_of_blanks : boolean;
begin
    cntr := 1;
    index := 0;
    repeat
        index := index + 1;
        out_of_blanks := eatblanks(input_str, cntr);
        charcntr := cntr;
        out_of_chars := eatchars(input_str, cntr);
        until (index = item) or out_of_blanks;
        theitem := copy(input_str, charcntr, (cntr - charcntr + 1));
        check_tail(theitem);
        get_nth_item := not out_of_blanks
    end;

{-----}
function theNextLine( var mydata : text ;
    var end_reached : boolean) : str132;
var
    the_line, throwaway : str132;
begin
    end_reached := false;
    theNextLine := '';
    repeat
        end_reached := eof(mydata);
        if (not end_reached) then
            begin
                readln(mydata,the_line);
                if dataflag then end_reached := (nulstr =copy(the_line,1,1));
            end;
        until ( semi_c () copy(the_line,1,1)) or end_reached;
        theNextLine := the_line;
    end;

{-----}
procedure get_those_nums (var mydata : text;
    xcol, ycol : integer;

```

```

                                var actualNums : integer);

const
    dwell = 10;
    one = '1.00000';
var
    theLine :str132;
    done : boolean;
    sigxcol, sigycol, i : integer;
begin
    write('Collecting data .');
    actualNums := 0;
    done := false;

    if xcol > 4 then sigxcol := xcol - 2 else sigxcol := 0;
    if ycol > 4 then sigycol := ycol - 2 else sigycol := 0;
    repeat
        actualNums := actualNums + 1;
        if (actualNums mod dwell) = 0 then write(dot);
        theLine := theNextLine(mydata, done);

        if (not done) then
            begin
                done := not(get_nth_item(theLine,
                                         xaray[actualNums], xcol));
                done := not(get_nth_item(theLine,
                                         yaray[actualNums], ycol));
            end;
        theLine := theNextLine(mydata, done);
        if (not done) then
            begin
                if sigxcol <> 0 then
                    begin
                        done := not(get_nth_item(theLine,
                                                  sigmx[actualNums], sigxcol));
                    end;
                if sigycol <> 0 then
                    begin
                        done := not (get_nth_item(theLine,
                                                  sigmy[actualNums], sigycol));
                    end;
            end;
        until done or (actualNums >= maxnums);
        actualNums := actualNums - 1;
        writeln(actualNums);
        writeln;
        if sigxcol = 0 then
            for i := 1 to actualNums do sigmx[i] := one;
        if sigycol = 0 then
            for i := 1 to actualNums do sigmy[i] := one;

end;
(-----)

```



```

function getColHeads(var theHeads : headaray;
                    var strcnt : integer) : boolean;
var
  lastitem, tempbool : boolean;
  myitem : str35;
  i : integer;
begin
  strcnt := 0;
  repeat
    strcnt := strcnt + 1;
    lastitem := get_nth_item(header, myitem, strcnt);
    theHeads[strcnt] := myitem;
  until not lastitem;
  strcnt := strcnt - 1;
  tempbool := strcnt > 0 ;
  if tempbool then { fix for PURE ENCODER }
  begin
    theHeads[4] := concat(theHeads[4], ' ', theHeads[5]);
    for i := 6 to strcnt do
      theHeads[i-1] := theHeads[i];
    strcnt := strcnt - 1;
  end;
  getColHeads := tempbool ;

end;
{-----}
procedure chooseCols(theHeads : headaray; hcnt: integer;
                    var xcol, ycol : integer );
var
  i : integer;
  allok : boolean;
begin
  repeat
    clrscr;
    for i := 1 to hcnt do
      writeln(i,dot,' ',theHeads[i]);
    write('Choose 2 columns = ');
    readln (xcol,ycol);
    allok := (xcol > 0 ) and (xcol <= hcnt);
    allok := (allok) and (ycol > 0) and (ycol <= hcnt);
  until allok;
end;
{-----}
procedure showdata( actcnt : integer; head1, head2 : str35);
var
  i : integer;
begin
  writeln( head1,' ',head2);
  for i := 1 to actcnt do
    writeln(xaray[i],' ',sigmx[i],' ',
            yaray[i],' ',sigmy[i]);

```

```

end;
{-----}
procedure make_dta (actcnt: integer);
const
    dwell = 10;
var
    thename : str20;
    i : integer;
    mydata : text;
begin
    thename := concat( fname, dta);
    writeln('Saving to: ', thename);
    write('Saving .');
    assign(mydata, thename);
    rewrite(mydata);
    writeln(mydata, headings[xcolumn]);
    writeln(mydata, headings[ycolumn]);
    for i := 1 to actcnt do
        begin
            if (i mod dwell) = 0 then write(dot);
            writeln(mydata, xaray[i], ' ', sigmx[i]);
            writeln(mydata, yaray[i], ' ', sigmy[i]);
        end;
    close(mydata);
    writeln; {cr for dots}
end;

{-----}
function sqaar ( x : real) : real;
begin
    sqaar := x * x ;
end;

{-----}
function getweight ( sig : str20) : str20;
var
    rsig, theweight : real;
    dummy : integer;
    wtstr : str20;
begin
    Val(sig, rsig, dummy);
    theweight := 1.0 / sqaar(rsig);
    Str(theweight:8:4, wtstr);
    getweight := wtstr;
end;

{-----}
function ymin( thearray : numarray ;
               nps : integer) : str35;
var
    tempreal, tempmin : real;
    code, i : integer;
    tempstrg : str35;
begin
    Val(thearray[1], tempmin, code);

```

```

    for i := 2 to nps do
      begin
        Val(thearray[i],tempreal,code);
        if tempreal ( tempmin then tempmin := tempreal;
      end;
      Str(tempmin, tempstrg);
      ymin := tempstrg;
    end;

    (-----)
function substrg ( a, b :str35) :str35;
var
  c : str35;
  tempa, tempb, tempc : real;
  code : integer;
begin
  Val(a, tempa, code);
  Val(b, tempb, code);
  tempc := tempa - tempb;
  Str(tempc, c);
  substrg := c;
end;
(-----)

procedure list_pts (ttlpts : integer);
const
  maxpars = 3;
  dwell = 10;
  parfile = 'FIT.PAR';
  comma = ',';
  czero = '0';
  one = '1.0000';
var
  coord, dummy, parcnt : integer;
  varfile : text;
  fitname, wtstr : str20;
  sigma, yback : str35;
  fitparm : array[1..maxpars,1..2] of str35;
{*****}
  procedure get_pars;
  var
    i : integer;
    pardata : text;
  begin
    assign(pardata, parfile);
    reset(pardata);
    for i:= 1 to maxpars do
      begin
        readln(pardata, fitparm[i,1]);
        readln(pardata, fitparm[i,2]);
      end;
    close(pardata);
  end;
end;

```

```

{*****}
begin
  if not yesorno('Save for Fit ? (y or n)? [n] ') then
    writeln('Save aborted! ',chr(7))
  else
    begin
      fitname := concat(fname,fit);
      writeln('Saving to : ',fitname);
      write('Saving .');
      yback := ymin(yaray, ttlpts);
      sigma := one;
      get_pars;
      assign(varfile,'fitfile.dat');
      rewrite(varfile);
      writeln(varfile,fname);
      close(varfile);
      assign(varfile, fitname);
      rewrite(varfile);
      writeln(varfile, ttlpts);
      writeln(varfile, ParamStr(2),comma, fitparm[1,2]);
      writeln(varfile, '1,0');
      writeln(varfile, '0.5');
      for coord := 1 to ttlpts do
        begin
          if (coord mod dwell) = 0 then write (dot);
          wtstr := getweight(sigmw[coord]);
          write(varfile,yaray[coord],',',wtstr,',');
          wtstr := getweight(sigmw[coord]);
          writeln(varfile,xaray[coord],',',wtstr);
        end;
      for parent := 2 to maxpars do
        writeln(varfile,fitparm[parent,1],comma,fitparm[parent,2]);
      writeln(varfile,'SigA,',sigma, czero);
      writeln(varfile,'SigB,', '0.0', czero);
      close(varfile);
      writeln; { or at the end of the dots }
    end;
end;
{-----}
{----- main loop control -----}
procedure maincontrol;
begin
  dataflag := false;
  errmsg[1] := ' All ok ';
  errmsg[2] := 'Hit an eof before getting to key word';
  fname := newfilename;
  open_the_file(the_file);
  writeln(' ... Searching for column headings ...');

  case go_to_head(the_file,header,angle) of

    true :
      begin

```

```

(   writeln(errmess[1]);
    writeln(header);      }

    if getColHeads(headings, headcnt) then
        begin
            ChooseCols(headings,headcnt,xcolumn, ycolumn);
            writeln('Reading from :',fname);
            if go_to_head(the_file,header, data) then
                begin
                    dataflag := true;
                    get_those_nums(the_file,xcolumn,ycolumn,arraycnt);
                end;

(           showdata(arraycnt, headings[xcolumn], headings[ycolumn]);)

            end
        else
            writeln('No headings found');
            close(the_file);
            make_dta(arraycnt);
(   list_pts(arraycnt); )
        end;

    false :
        begin
            writeln(errmess[2]);
            close(the_file);
        end;

    end; {case}

end;

(-----checkfor all params -----)
begin
    if ParamCount = 2 then
        maincontrol
    else
        {Abort }
        writeln ('Usage: [file prefix] [number of fit iterations]');
    end.{filetest}

```

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