Real-time computer-optimized electron coincidence spectrometer

Andrew J. Murray, Brian C. H. Turton,[a] and Frank H. Read
Department of Physics, Schuster Laboratory, Manchester University, Manchester, M13 9PL, United Kingdom

An electron coincidence spectrometer utilizing real-time optimization and control by a standard IBM 80286 personal computer is described. Details of the system hardware and software are presented together with a description of the optimization routine adopted for maintaining the tuning of the spectrometer and data acquisition. Data collected by the computer-controlled spectrometer for (*e,2e*) coincidence experiments are also presented.

I. INTRODUCTION

Experiments utilizing electron excitation of atoms and molecules have been of interest since the early days of atomic physics. The first experiments in arc discharge tubes and vapor cells measured properties of either the fluorescence radiation emanating from the target or electron current variations as the electrons passed along the tube. As measurement technology improved these were followed by atomic/molecular beam experiments in vacuum chambers, where the incident electron beam energy could be accurately controlled by the use of electrostatic or magnetic lenses and where individual photons, electrons or ions arising from the interaction region could be detected.

The most detailed experimental results are obtained when two or more particles resulting from the reaction are detected in coincidence and correlations between these particles are measured. The first coincidence experiments in atomic physics were implemented in 1969 by Imhof and Read[1] who measured the fluorescence decay of electron-excited valence states of helium and by Ehrhardt et al.[2] in the same year who measured correlations existing between the two electrons resulting from the electron impact ionization of helium. The coincidence technique has since been applied principally to two groups of experiments involving electron impact. In the first, angular and energy correlation between the resulting electrons following electron impact ionization are measured in the so-called (*e,2e*) experiments (e.g., Ehrhardt *et al.*,[3] and references therein). In the second type of coincidence experiment, the incident electron excites a valence state of the target, which relaxes to a lower state by emitting a photon. This photon is detected in coincidence with the scattered electron and information is obtained by measuring either the angular distribution of the correlated photon as in the experiments of Eminyan *et al.*[4] or the coherences of the resulting coincident fluorescence are determined.[5,6]

The principal difficulty associated with these experiments is the relatively low coincidence count rate which can vary from a few events per second to only a few per hour. This places stringent conditions upon the stability of the experiment. To achieve reliable, reproducible results

often requires the operator to maintain close surveillance of the experiment to allow for any drifts in the running of the apparatus. The computer-optimized spectrometer described here deals with these difficulties independently of operator assistance by allowing for any variation of the experimental conditions with time. Other advantages of computer-controlled optimization are that any number of voltages can be varied simultaneously and that the optimization procedure can be repeated frequently during the course of an experiment to give results that are more consistent and reliable than those obtained under manual control.

The principle of computer control and optimization can also be applied to other types of spectrometer, as long as a figure of merit can be obtained for the function to be optimized. As an example, the resolution of the present spectrometer has been optimized to yield the best statistics when obtaining Fano profiles of resonance states in helium, by applying a figure of merit based upon the ratio of the profile intensity to profile width. The weighting given to the adjustable parameters defining the figure of merit will depend upon the particular application, as well as upon the tuning profile of the individual spectrometer.

This paper is divided into four principal parts. First, the spectrometer and the pulse techniques used to obtain the coincidence signal are described. The hardware interfacing the IBM 80286 PC to the spectrometer is then considered, following which the software controlling the experiment is outlined. Finally, correlated coincidence results from the computer optimized spectrometer are presented and the technique reviewed.

II. THE ELECTRON COINCIDENCE SPECTROMETER

The electron coincidence spectrometer was initially designed and constructed to measure angular and energy correlations between low-energy electrons emerging from near-threshold electron impact ionization of helium.[7] These experiments were conducted in the perpendicular plane (Fig. 1), defined as the plane where the two correlated electrons emerge perpendicular to the momentum vector of the incident electron beam, and were designed to test the theories of the Wannier model for near-threshold ionization processes.[8]

A number of modifications to the original spectrometer design as described in Hawley-Jones *et al.*[7] have been im-

[a] School of Electrical, Electronic and Systems Engineering, University of Wales College of Cardiff, Cardiff, Wales, CF1 3YH, United Kingdom.
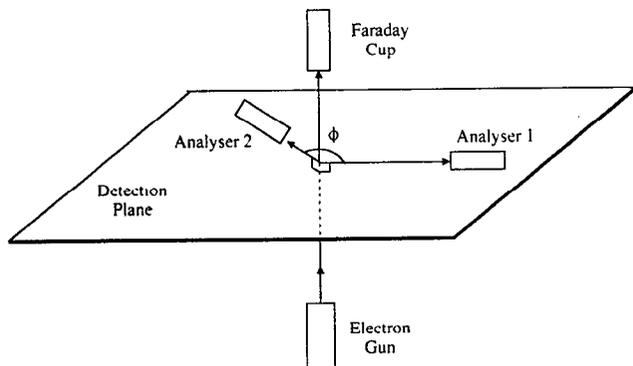
FIG. 1. Perpendicular plane geometry, for which the momentum vector of the incident electron beam is perpendicular to the momentum vectors selected for the analyzed electrons.

plemented. Figure 2 is a schematic of the existing apparatus showing the spectrometer configured in the perpendicular plane geometry. The spectrometer is mounted vertically on a 30 mm 310 grade stainless-steel flange supported by a 1500 mm vacuum chamber, which is pumped by a 500 ℓ/s Balzers turbomolecular pump, achieving a background residual pressure of 1.5×10^{-8} Torr. To minimize external magnetic fields the chamber is shielded by 3-mm-thick μ-metal internally and externally.

The electron gun incorporates two triple aperture electrostatic lenses and has an energy resolution given by the thermal energy distribution of the tungsten filament source, ~ 600 meV. The electron energy can be varied from 20 to 300 eV and the gun is capable of supplying up to 4 μA of current focused to a 1 mm diameter at the interaction region. 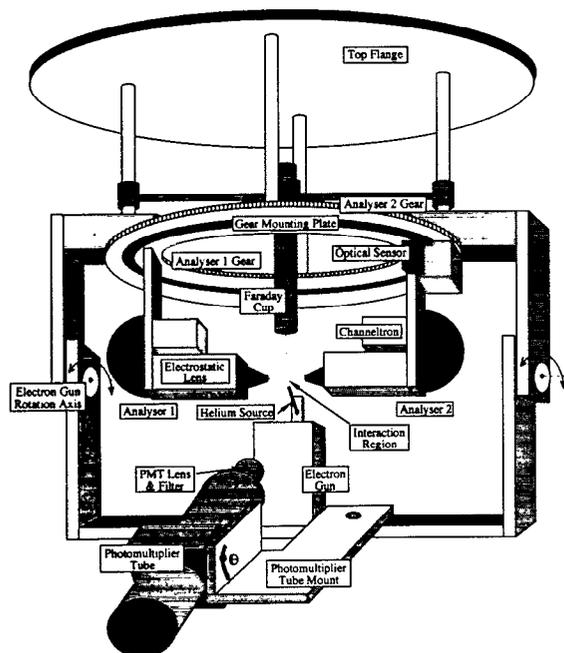The gun, photomultiplier tube, and atomic beam source are mounted so as to rotate from the perpendicular plane geometry to the plane of analyzer rotation. The atomic beam intersects the electron beam trajectory at 45°, this being the optimum angle at these two extremes. The Faraday cup collects all electrons passing directly through the interaction region and is either mounted as shown in Fig. 2 or is connected to the atomic beam support.

The interaction region is focused onto an EMI 9789QB photomultiplier tube to allow the electron gun to be tuned independently of the tuning of either of the scattered electron energy analyzers. The focusing lens is a 25 mm $f1.2$ plano-convex glass lens covered with a fine tungsten mesh to eliminate surface charging. A 1 mm aperture and an optical filter placed directly in front of the photomultiplier tube passes helium radiation at 450 nm. This wavelength is chosen as it allows the aperture to be visibly back-focused onto the interaction region. This is accomplished by placing a light source inside the photomultiplier tube housing behind the aperture and adjusting the lens position so as to image the aperture at the interaction region. The photomultiplier tube is cooled by passing nitrogen gas boiled off liquid nitrogen through copper coils encircling the housing.

The hemispherical electron analyzers rotate in the horizontal plane via internal 10:1 gears coupled to external stepper motors via 10:1 stepdown gearboxes. The input electrostatic lenses to the hemispheres are triple element cylindrical lenses constructed of molybdenum. Following energy selection in the hemispheres the electrons are detected by a Mullard X919BL channeltron. The analyzers are prevented from colliding by optical interrupters constructed from hermetically sealed infrared SD54433 phototransistors and TEMT88PD light-emitting diodes placed on either side of analyzer 2. These interrupters sense the presence of analyzer 1 and shut down the stepper motor drive units external to the spectrometer. Additional interrupters mounted from the spectrometer support struts prevent the analyzers from colliding with the electron gun when nonperpendicular plane geometries are selected.

All surfaces of the spectrometer that surround the electron beam are constructed from molybdenum, while the spectrometer mountings are carbon-coated 310 stainless steel. Connections to all electrostatic lens elements and deflectors are via shielded 0.5 mm color coded PTFE coated advance wire. The channeltron and photomultiplier tube signal and high-voltage lines are doubly shielded PTFE coated RG188A/U co-axial cable. Vacuum pressure is monitored by a Vacuum Generators ion gauge head connected to a VG IGP 3 controller.

A schematic of the electron detection and pulse timing circuitry is given in Fig. 3. The channeltron high voltages are supplied by two Brandenberg Alpha Series II 5 kV supplies via low-pass filters located at the spectrometer feedthroughs, while the photomultiplier tube high voltage is supplied by a Brandenberg 475R 2 kV supply. The photomultiplier produces 10 ns negative going pulses of average height ~ 200 mV which are fed directly to an ORTEC 473A discriminator for noise discrimination. The
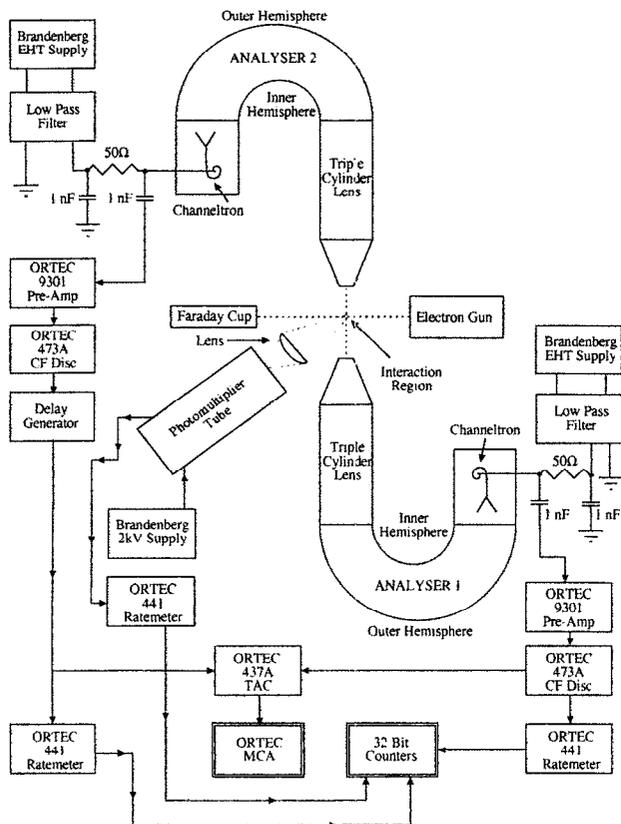

FIG. 2. Spectrometer configured in the perpendicular plane.

FIG. 3. Coincidence timing and pulse circuitry.

FIG. 4. IBM 80286 PC hardware interface to the spectrometer.

resulting pulses are fed to an ORTEC 441 ratemeter for counting. The 10-ns-wide negative going channeltron pulses of average height ~ 30 mV are initially amplified by ORTEC 9301 $10\times$ preamplifiers located directly at the vacuum feedthrough before being sent via doubly shielded Belden RG58A/U coaxial cable to a pair of ORTEC 473A constant fraction discriminators. The discriminators are located in separate NIM crates to increase isolation, thereby decreasing common mode noise on the signals which can produce spurious coincidence counts. The channeltron count rates are monitored by separate ORTEC 441 ratemeters. Fast NIM pulses from the discriminators are fed to an ORTEC 437A time-to-amplitude converter (TAC) via appropriate delay lines, allowing the coincidence signal to fall within the time domain selected by the TAC. The TAC output is sent to an ORTEC multichannel analyzer (MCA) located onboard the main IBM 80286 PC bus, while the outputs from the ratemeters are fed to 32-bit counters also located on the main PC bus. The coincidence timing signal approximates a Gaussian function with an overall timing resolution dictated by the energy resolution of the analyzers, the channeltron pulse height characteristics, preamplifier rise times, and discrimination electronics. Typically, the measured full width at half maximum of the coincidence signals observed is ~ 8 ns.

III. THE COMPUTER HARDWARE INTERFACING

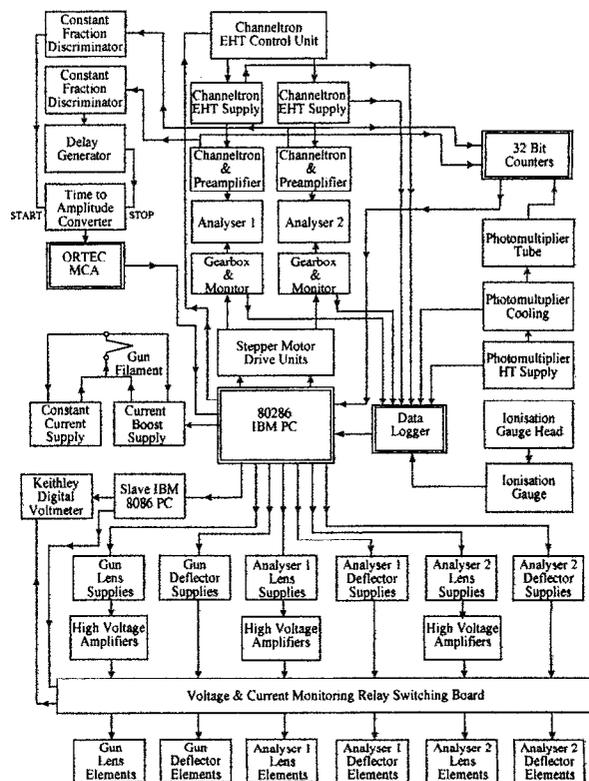Figure 4 is a block diagram of the hardware interface between the computer and the spectrometer. At the heart of the system is the main IBM 80286 PC which controls the spectrometer and receives all information about the system status from the monitors. The voltages controlling the electrostatic lenses and deflectors in the gun and analyzers are supplied by separate optically isolated active supplies as detailed elsewhere.[9,10] 12-bit digital-to-analog converter (DAC) cards either directly feed the lens and deflector elements or are routed through stable high-voltage amplifiers before being fed to the spectrometer. A 70 relay switching board allows either the current or voltage on a selected lens element to be measured by a Keithley digital volt/current meter which is addressed via an IEEE-488 bus by the slave 8086 PC. The slave PC is in turn controlled by the main PC via an RS-232 serial line.

The analyzer angles are controlled by Compumotor intelligent stepper motor drive units via 100:1 stepdown gears, and are monitored by ten-turn potentiometers located in the drive shafts external to the spectrometer. The potentiometer voltages are monitored by a Blue Chip AIP-24 24 channel ADC datalogger located on the main PC bus. This datalogger also monitors the Brandenberg EHT supplies to the channeltrons and PM tube, the temperature of the PM tube and the vacuum pressure in the system via appropriate buffer amplifiers. The channeltron EHT supplies are controlled by serial driven DAC cards which are addressed by the main 80286 PC. Pulses from the channeltrons and PM tube are monitored by an AMD 9513 based 32-bit counter board on the main PC bus, and the TAC output is sent directly to the MCA card installed in the main PC. Finally, the constant current supply to the

electron gun filament contains a current boost circuit that allows small increased current to be supplied to the gun during spectrometer tuning.

IV. THE COMPUTER SOFTWARE CONTROL

The software controlling the electron coincidence spectrometer is written to address specific tasks unique to the coincidence experiment as well as tasks common to all forms of computer control of electron spectrometers. The 80286 PC controls all aspects of the tuning of the spectrometer electrostatic lenses and deflectors during operation, and in addition controls the position of the analyzers as they rotate around the interaction region in order to build up a coincidence angular correlation function. A total of seventeen voltages, corresponding to five lens elements and six deflector elements in the gun and one lens element and two deflector elements in each analyzer, are optimized by the computer. A number of inbuilt system status checks allow the data accumulation to be halted should problems arise during operation, and act as additional protection for the channeltrons should the system pressure rise above safe levels. Inbuilt software protection prevents the analyzers from colliding either with each other or with the electron gun, in addition to the hardware protection measures discussed in Sec. II. The data from the MCA card, 32-bit counter card, datalogger, and 8086 slave PC are stored both on an internal 40MB hard disk as well as onto a 5.25 in. floppy disk during the experiment as data are accumulated.

Figure 5 is a block diagram of the software control routines. The method chosen for optimization of the spectrometer uses a modified form of the simplex technique[11,12] and as with all techniques reaches the best conditions most quickly when given a starting position close to the optimum. The spectrometer is therefore initially set up either manually or by using the operating conditions found by a previous optimization survey, and the required running conditions for the experiment are read from a data file. A flag option either calibrates the DAC cards, thus allowing for any amplifier variation, or the initial voltages at setup are directly loaded to the lens and deflector elements. The system status is then read from the datalogger and any faults (e.g., EHT supplies out of range, vacuum pressure unacceptable, etc) are corrected.

The coincidence experiment measures the intensity of the angular correlation function as the analyzer angular positions are varied around the detection plane (Fig. 1). Initially, the electron gun is optimized to electron beam current as measured by the Faraday cup, which involves the variation of four aperture lens voltages and four pairs of deflector voltages. The electron beam is then steered and focused using a total of four lens and deflector voltages onto the gas jet, defining a 1 mm volume at the interaction region as detected by the photomultiplier tube. This optimization procedure is followed whenever the energy or direction of the electron beam are changed, and typically takes about 10 min to complete.

Following optimization of the electron gun onto the interaction region, the system status is rechecked and the
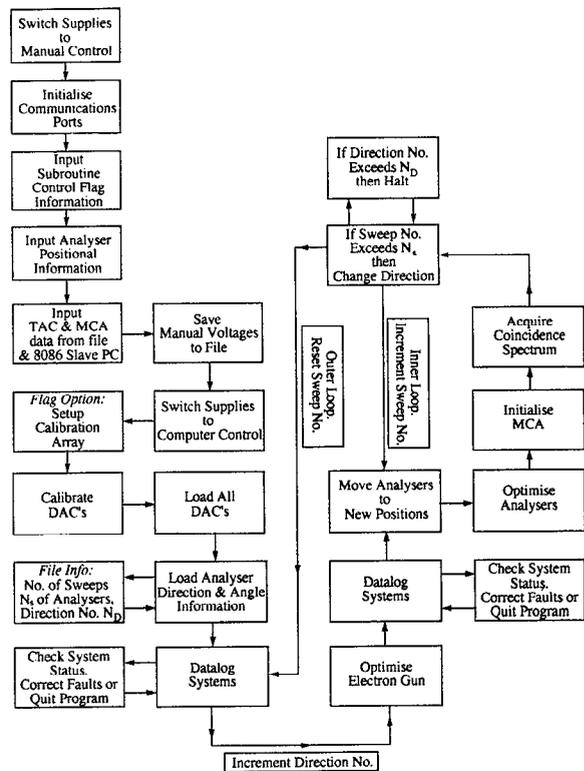

FIG. 5. Computer software control.

analyzers are moved to their initial positions. Each analyzer is focused onto the interaction region which involves the variation of a total of six lens and deflector voltages, after which the MCA is initialized. A coincidence spectrum is then accumulated for a predetermined time, the system being logged every 50 s to allow later analysis should anomalies be detected in the data. At this point the inner loop takes command. The analyzers are moved around the detection plane, optimized at each angle and coincidence data are collected.

Once the number of angles at which data is collected exceeds a predetermined value N_s, the outer loop once more takes control and the whole system is checked and reoptimized. Any long-term drifts in the apparatus are therefore accounted for by accumulating data at each scattering angle for a short time. During normal operation the analyzers sweep back and forth around the detection plane many times, the angular correlation function gradually emerging from the accumulated data.

V. THE SIMPLEX OPTIMIZATION ROUTINE

The software routine chosen to optimize the coincidence spectrometer uses a modified simplex algorithm based upon the routine of Nelder and Mead.[11] This technique has been found to be robust in the presence of noise and statistical fluctuations as are present on the outputs of channeltrons and photomultipliers[13] and has the additional advantage that the form of the parameter to be optimized
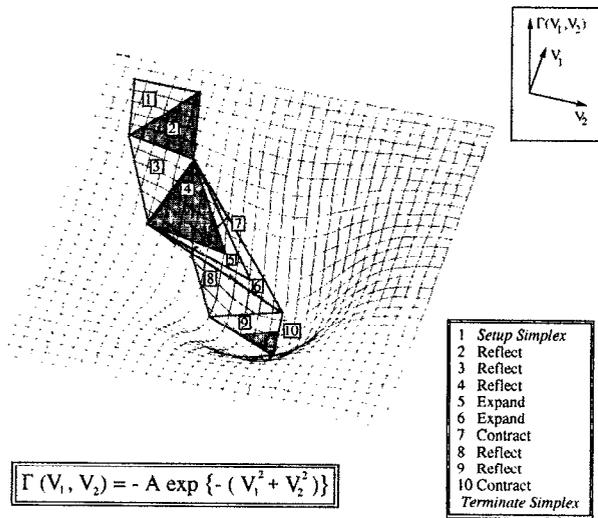
FIG. 6. Simplex converging onto the minimum of the function $\Gamma(V_1,V_2) = -A \exp[-(V_1^2 + V_2^2)]$.

as a function of the selected variables is not required. The routine is multidimensional, allowing optimization over a space comprising in this case the lens and deflector element voltages V_i as a basis.

A simplex in N dimensions is a geometric polygon with $N + 1$ interconnecting vertices and so in two dimensions the simplex is a triangle. As an example of the simplex technique, Fig. 6 shows the two-dimensional Gaussian function

$$\Gamma(V_1,V_2) = -A \exp[-(V_1^2 + V_2^2)]. \qquad (1)$$

In this case, the optimum point is given as the minimum of the function and Fig. 6 shows a 2D simplex converging onto the minimum of $\Gamma(V_1,V_2)$. The starting simplex chosen here is purely arbitrary, and the designated steps 1–10 will vary depending upon this chosen starting point. The routine moves the simplex through a series of steps consisting mostly of reflections of the worst function value vertex through the opposing "face." The routine expands the simplex whenever it can to reduce the number of required functional evaluations, and can also contract the simplex around the best point if necessary. Combinations of reflection, expansion, and contraction allow the simplex to find the minimum of the function $\Gamma(V_1,V_2)$. It is noted that the functional form of $\Gamma(V_1,V_2)$ is not required in order to converge onto the minimum.

Experimentally, when optimizing a parameter using N voltages, the routine sets up $N + 1$ points which comprise the initial voltage settings and points set predetermined step sizes from this point along the chosen voltage element as a basis. The initial step size along any basis is dictated by the sensitivity of the measured parameter to that particular element. The optimization routine then proceeds as in the example above. Termination of the routine occurs if either the calculated voltage step size in all dimensions is smaller than the associated DAC single-bit voltage step or if a predetermined number of iterations is exceeded. A second
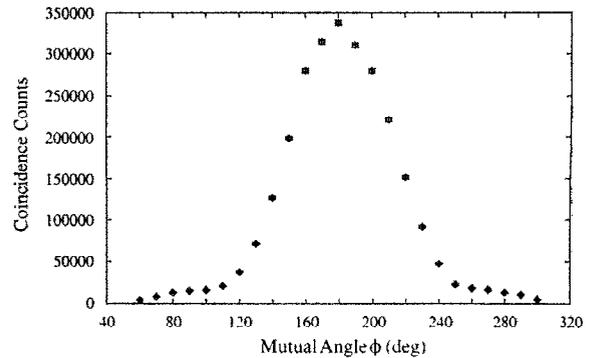

FIG. 7. Perpendicular plane coincidence angular correlation function at 34.6 eV incident energy using a helium target. The energy of the scattered and ejected electrons is 5 eV.

optimization attempt is then carried out from the point of the first success in order to test for the possible existence of deeper minima elsewhere.

VI. COINCIDENCE RESULTS FROM THE OPTIMIZED SPECTROMETER

The optimized coincidence spectrometer has been operating almost continuously for one year, with only minimal operator assistance. Initial tests showed that the computer optimization produced coincidence yields 20%–50% higher than those obtained manually. This improvement arises partly because several electrostatic elements can be varied simultaneously. Since these initial tests the spectrometer has run for up to four weeks without operator assistance and has produced reliable, reproducible results in a far shorter period of time than would have been possible if completely under manual control, since the spectrometer accumulated data continuously 24 h per day. The results are statistically more consistent and reliable than similar results obtained under manual control using the same spectrometer.[14] Figure 7 shows an example of the angular correlation obtained scattering from a helium target at an energy of 34.6 eV, whereas Fig. 8 shows the angular correlation at an incident energy of 74.6 eV. In
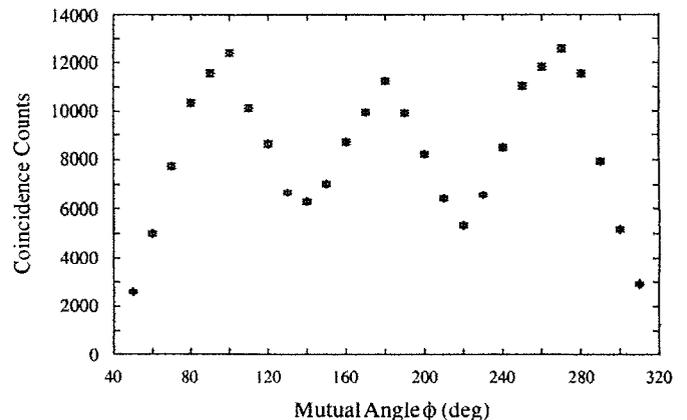

FIG. 8. Symmetric energy perpendicular plane coincidence angular correlation function at 74.6 eV incident energy using a helium target. The energy of the scattered and ejected electrons is 25 eV.
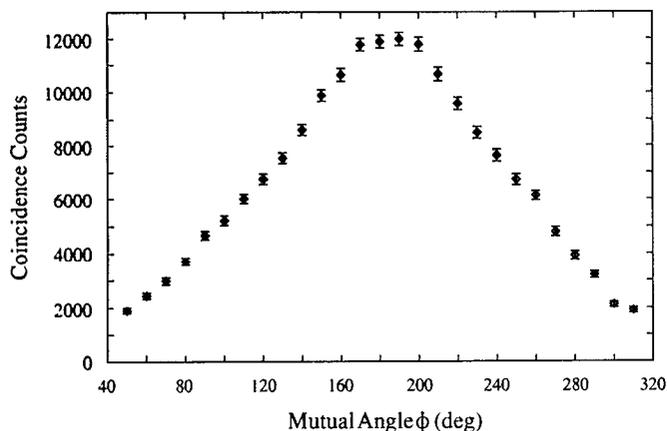
FIG. 9. Nonsymmetric energy perpendicular plane coincidence angular correlation function at 74.6 eV incident energy using a helium target. The energies of the scattered and ejected electrons are 5 and 45 eV.

both of these examples the scattered and ejected electrons resulting from the reaction were detected with equal energy, and the evolution of the correlation function with increasing energy is clearly evident. The symmetry of the correlation function around $\phi = 180°$ is necessary from the experimental symmetry in the perpendicular plane, and these results indicate that the spectrometer performs reliably over the 230° sweep of the detection plane used to obtain these results. The results accumulated for the complete angular correlation survey using different incident and collection energies also shows this symmetry, reflecting the reliable nature of the optimization technique.

A detailed survey of the perpendicular plane geometry angular correlation function for both symmetric and nonsymmetric energies of the detected electrons has now been conducted for a range of incident energies from 10 to 80 eV

above the ionization threshold in helium.[15] Figure 9 shows the result obtained for the nonsymmetric energy case at 74.6 eV incident energy, where the scattered and ejected electrons were detected with energies of 5 and 45 eV, respectively. This result may be contrasted with the results for the symmetric case presented in Fig. 8, and indicate that a quite different scattering mechanism is occurring.

ACKNOWLEDGMENTS

[1] R. E. Imhof and F. H. Read, Chem. Phys. Lett. 3, 652 (1969).
[2] H. Ehrhardt, M. Schulz, T. Tekaat, and K. Willmann, Phys. Rev. Lett. 22, 89 (1969).
[3] H. Ehrhardt, K. Jung, G. Knoth, and P. Schlemmer, Z. Phys. D 1, 3 (1986).
[4] M. Eminyan, K. B. MacAdam, J. Slevin, and H. Kleinpoppen, J. Phys. B 7, 1519 (1974).
[5] M. C. Standage and H. Kleinpoppen, Phys. Rev. Lett. 36, 577 (1976).
[6] A. J. Murray, C. J. Webb, W. R. MacGillivray, and M. C. Standage, Phys. Rev. Lett. 62, 411 (1989).
[7] T. J. Hawley-Jones, F. H. Read, S. Cvejanović, P. Hammond, and G. King (unpublished).
[8] F. H. Read, Electron Impact Ionization, edited by G. Dunn and T. Märk (Springer, Berlin, 1985), pp. 42–88.
[9] S. K. Howell, J. Phys. E. 20, 288 (1987).
[10] N. J. Bowring (unpublished).
[11] J. A. Nelder and R. A. Mead, Comput. J. 7, 308 (1965).
[12] S. K. Howell, N. J. Bowring, and T. D. S. Hamilton, J. Phys. E 20, 293 (1987).
[13] B. C. H. Turton, Ph. D. thesis, Victoria University of Manchester, 1991.
[14] M. B. J. Woolf, Ph. D. thesis, Victoria University of Manchester, 1989.
[15] A. J. Murray, M. B. J. Woolf, and F. H. Read (unpublished).