ELASTIC AND INELASTIC ELECTRON SCATTERING BY ATOMS AND MOLECULES IN THE BACKWARD DIRECTION

M.Zubek

Department of Physics of Electronic Phenomena, Technical University, 80-952 Gdańsk, Poland

Progress made recently in studies of electron scattering by atoms and molecules at large scattering angles up to 180^0 is reported. Results obtained at scattering angles from 120^0 to 180^0 for elastic and inelastic electron scattering using the magnetic angle-changing technique are discussed.

1. Introduction

Systematic experimental studies of elastic and inelastic electron scattering by atomic and molecular targets for scattering angles in the backward hemisphere $90^0 - 180^0$ became possible only recently with the development of new techniques, the electron – mirror spectrometer [1] and the magnetic angle – changing technique [2,3]. Such studies have not been carried out previously although some attempts have been made to observe elastic scattering of electrons at 180^0 [4,5] or to measure elastic cross sections integrated over the backward hemisphere [6]. Investigations of electron scattering in the backward direction bring important information and here several reasons for studying backward scattering can be pointed out. The differential cross sections (DCS) for elastic and inelastic scattering may be determined over the whole scattering angle range from 0^0 to 180^0 without recourse to extrapolation techniques. The angular dependence of the DCS in the electronic excitation depends on the symmetry of the state being excited and in the scattering with formation of negative-ion resonances is directly related to the symmetry of the resonance state.

From the DCS obtained over the complete scattering sphere integral cross section $\sigma(E)$ and momentum transfer cross section $\sigma_m(E)$ at a given electron energy E may be obtained from the integration

$$\sigma(E) = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega}(E,\theta)\sin\theta d\theta \quad , \qquad (1)$$

$$\sigma_m(E) = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega}(E,\theta)(1-\cos\theta)\sin\theta d\theta \ ,(2)$$

where $\frac{d\sigma}{d\Omega}(E,\theta)$ is the DCS at an electron energy E and a scattering angle θ. As is seen from (2) scattering in the $90^0 - 180^0$ angular range has a greater weighting factor in its contribution to σ_m than forward scattering. It is also interesting to point out that the determination of the cross section according to (1) and (2) would give values with higher accuracy especially for the inelastic electron scattering eliminating the uncertain extrapolation procedures used at present in most of the experimental measurements.

Measurements of elastic scattering in the backward direction are also of interest in the partial wave description of scattering and for the determination of the phase shifts. This is more complex for heavier atoms (Xe, Hg) where more partial waves contribute to the electron scattering. Here the DCS is given by

$$\frac{d\sigma}{d\Omega} = |f(E,\theta)|^2 \quad , \qquad (3)$$

where the scattering amplitude $f(E,\theta)$ for the spin independent scattering is expressed by

$$f(E,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta) \ .(4)$$

In (4) k is the wave number for the incident electron energy E, δ_l is the phase shift for given angular momentum l and P_l are respective Legendre polynomials. At the scattering angle of 180^0 all partial waves that contribute to the scattering are included in (4) with their Legendre polynomials (modulus) equal to 1.

Furthermore, at 180^0 (as well as at 0^0) scattering angle it is predicted, on the grounds of theoretical group considerations [7,8], that the DCS for electronic excitation of "parity unfavoured" transitions in atoms e.g. $^1S_g \rightarrow {}^3P_g$ and of certain transitions in molecules e.g. $\Sigma^- \rightarrow \Sigma^+$ is equal to zero. This new "selection rule" would allow the identification of the symmetries of excited states on the basis of their angular behaviour in electron scattering at and close to 180^0. Finally it is also expected that the observation of electron scattering in the backward direction would enable new resonance and cusp features to be detected.

2. Elastic electron scattering

The absolute differential cross sections (DCS) for elastic electron scattering in nitrogen (N_2) obtained at incident electron energies of 5 and 6eV, in the angular range from 120° to 180°, are shown in Figs. 1 and 2 respectively. The most recent experimental data obtained for lower scattering angles and the results of theoretical calculations are also shown for comparison. The high scattering angle data obtained using the magnetic angle – changing technique [9] agree well with the low scattering angle results in the overlap region and combine to give elastic cross sections over the angular range from 20° to 180°.

For the theoretical results at 5 eV (Fig. 1) the hybrid theory calculations [11] which combine vibrational close – coupling with the adiabatic nuclei approximation show the best agreement with the experimental cross section although they are about 20 – 30% higher in magnitude. The R-matrix calculations [12] overestimate the DCS in the forward direction below 50° and the Schwinger multichannel results [13] in the region of scattering angle above 100° deviate from the experimental DCS. These discrepancies between theoretical and measured DCS have been attributed to inadequate representation of the long-range and short-range correlation interaction for low- and high-angle scattering respectively [9]. At 6 eV (Fig. 2) the experimental cross sections are compared with the only available theoretical results which are converged vibrational close – coupling calculations [14]. There is very good agreement between both sets of data above 60° but at lower scattering angles the calculated values overestimate the experimental elastic DCS by about 40% .

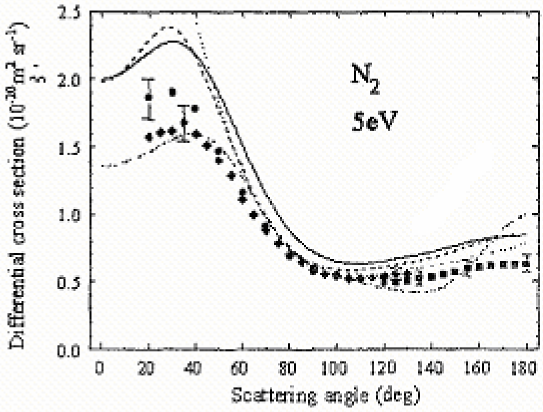

Fig. 1. Differential cross sections for elastic electron scattering in nitrogen at an incident electron energy of 5 eV. Experimental results: [17] – open circles, [14] – full diamonds, [9] – full squares. Theoretical results : [11] – full line, [12] – dotted line, [13] – dashed-dotted line, [14] – dashed line

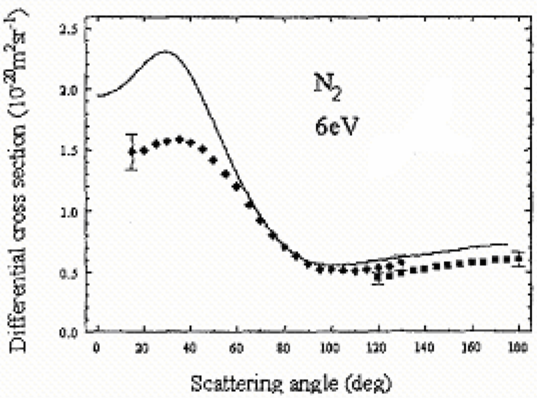

Fig. 2. Differential cross sections for elastic electron scattering in nitrogen at an incident electron energy of 6 eV. Experimental results: [14] – full diamonds, [21] – full squares. Theoretical results: [14] – full line.

Interesting results have been obtained for sulphur hexafluoride (SF_6) molecules which unlike nitrogen have spherical symmetry and high dipole polarizability. The DCS for elastic scattering of electrons by sulphur hexafluoride measured for scattering angles between 130° and 180° at the incident energy of 5eV are shown in Fig. 3 together with the DCS for lower scattering angles obtained in two different laboratories. These results have been obtained again by the magnetic angle – changing technique using a modified design of the source of the localized magnetic field [15]. The cross section decreases with increasing scattering angle above 120° and its lowest value occurs for backscattering at 180°. The close – coupling calculations [16] reproduce the general angular behaviour of the experimental cross section. However for backward scattering they predict a DCS which is higher by a factor of about 2.

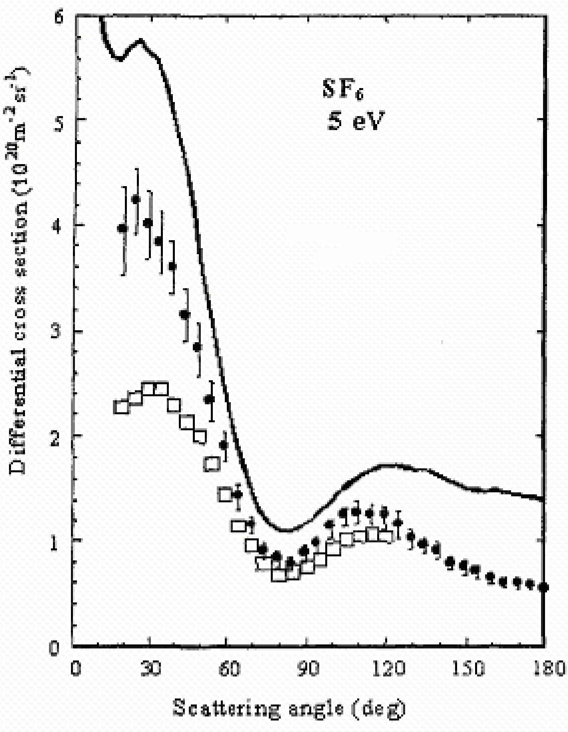

Fig. 3. Differential cross sections for elastic electron scattering in sulphur hexafluoride at an incident electron energy of 5 eV. Experimental results: [15] - full circles, [18] - open squares. Theoretical results: [16] full line.

3. Resonance electron scattering

The magnetic angle-changing technique have been used to make the first observation of the resonance structures corresponding to the $2s^2\ ^2S$ state in He^- and the $np^5(^2P_{3/2,1/2})(n+1)s^2$ states in Ne^-, Ar^-, Kr^- and Xe^- in elastic scattering near 180° [3]. The results obtained for the $4p^5(^2P_{3/2,1/2})5s^2$ resonance in krypton are shown in Figs. 4 and 5 respectively. Also shown are theoretical profiles (full curves) which have been obtained from a fitting procedure using the partial waves cross section formulas for the spin – dependent scattering. In the angular range above 130° the shapes of the structures stay approximately unchanged with increasing scattering angle. Also the magnitude of the resonance structures, measured with respect to the non – resonant background, is approximately constant. The $^2P_{1/2}$ structure (Fig. 5) is symmetric and has smaller intensity than the $^2P_{3/2}$ structure and is also broader. These features of the $^2P_{1/2}$ resonance are related to its position above the first two $4p^55s$ J = 2,1 excited states of krypton. The above backscattering measurements allowed the natural width of the $^2P_{1/2}$ resonance to be determined to be 30 ± 4 meV.

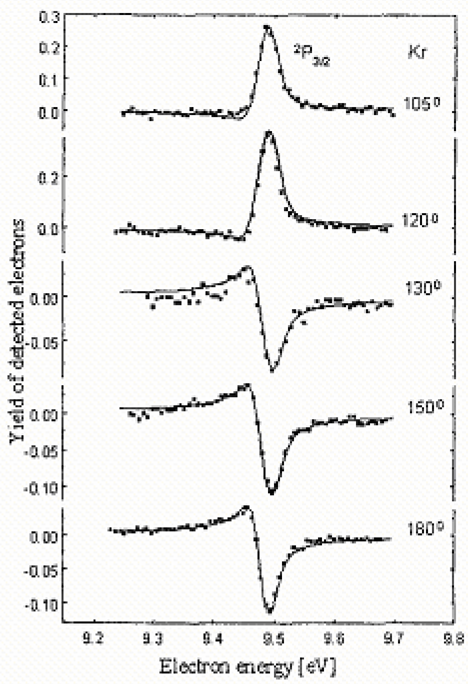

Fig. 4. Resonance structures of the $^2P_{3/2}$ state in the elastic electron scattering by krypton at indicated scattering angles [3]. Full lines give the fitted theoretical profiles.

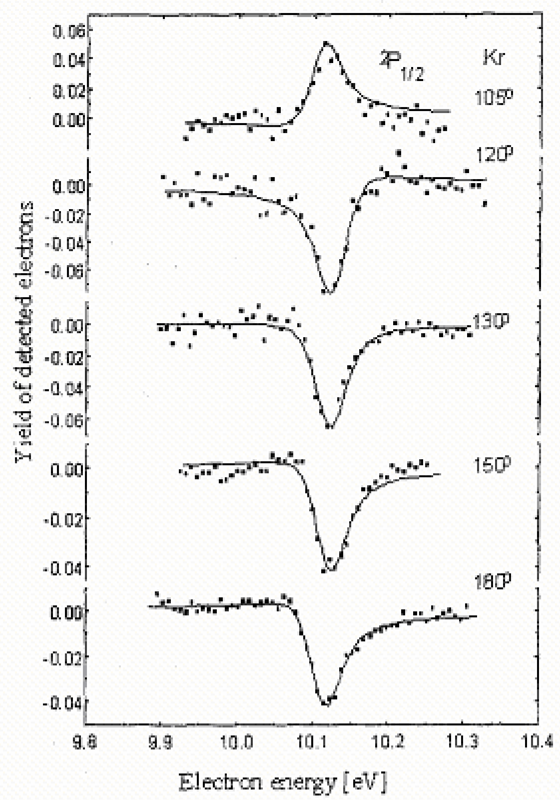

Fig. 5. Resonance structures of the $^2P_{1/2}$ state in the elastic electron scattering by krypton at indicated scattering angles [3]. Full lines give the fitted theoretical profiles.

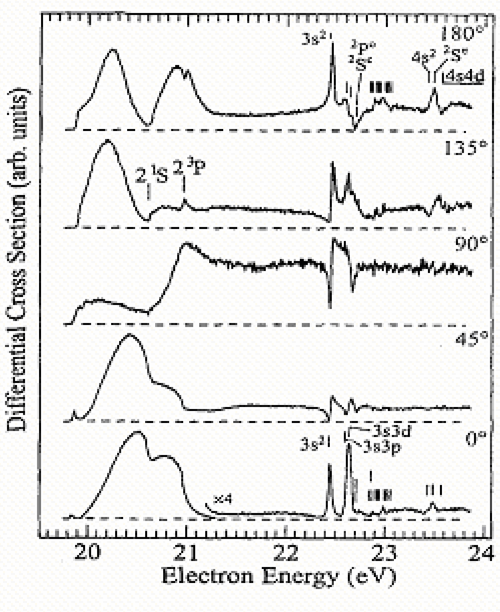

Fig. 6. Differential cross sections for excitation of the 2^3S state of helium at given scattering angles [19]. Vertical lines above the spectra indicate calculated resonance energies [20]. The 2^1S and 2^3P excitation thresholds are also shown.

Resonance processes of the negative-ion states decaying to excited states of atoms have been observed for the first time for the backward scattering in studies of excitation of the $n = 2$ states of helium [1, 19]. Fig. 6 compares the DCS recorded at 180° using the magnetic angle-changing technique with that obtained at lower scattering angles without use of a magnetic field [19]. A dramatic change in the shape of resonant structures with scattering angle is clearly seen which gives more information on the highly-excited ridge resonances. In particular, in the 180^0 spectrum a dip is observed at 22.69 eV which coincides with the position of the $^2P^o$ and $^2S^e$ resonances determined by theoretical calculations [20]. In this spectrum of notice is a cusp structure at the 2^3P excitation threshold which has a shape of a dip followed by a peak. A cusp at the 2^3P threshold but displaying a different shape is also detected in the 135^0 spectrum.

Acknowledgements

I would like to acknowledge with pleasure my collaborators who contributed to the presented work: J.Channing, G.C.King, B.Mielewska and F.H.Read.

References

1. K.R.Asmis, M.Allan, *J. Phys. B* **30,** 1961 (1997).
2. F.H.Read, J.M.Channing, *Rev. Sci. Instrum.* **67,** 2372 (1996).
3. M.Zubek, B.Mielewska, J.Channing, G.C.King, F.H. Read, *J. Phys.B* **32,** 1351 (1999).
4. P.D.Burrow, L.Sanche, *Phys. Rev. Lett.* **28,** 333 (1972).
5. D.Roy, P.D.Burrow, *J. Phys. E* **8,** 273 (1975).
6. J.B.Greenwood, I.D.Williams, B.Srigengan, W.R.Newell, J.Geddes, R.W.O'Neill, *J. Phys. B* **28.** L307 (1995).
7. D.C.Cartwright, S.Trajmar, W.Williams, D.L.Huestis, *Phys. Rev. Lett.* **27**, 704 (1971).

8. W.A.Goddard III, D.L.Huestis, D.C.Cartwright, S. Trajmar, *Chem. Phys. Lett.* **11,** 329 (1971).
9. M.Zubek, B.Mielewska, G.C.King, *J. Phys. B* **33** (in press).
10. T.W.Shyn, G.R.Carignan, *Phys.Rev.A* **22,** 923 (1980).
11. N.Chandra, A.Temkin, *Phys. Rev. A* **13,** 188 (1976).
12. C.J.Gillan, O.Nagy, P.G.Burke, L.A.Morgan, C.J.Noble, *J. Phys. B* **20,** 4585 (1987).
13. W.M.Huo, M.A.P.Lima, T.L.Gibson, V.McKoy, *Phys. Rev. A* **36** 1642 (1987).
14. W.Sun, M.A.Morrison, W.A.Isaacs, W.K.Trail, D.T.Alle, R.J.Gulley, M.J.Brennan, S.J.Buckman, *Phys.Rev.A* **52,** 1229 (1995).
15. H.Cho, R.J.Gulley, S.J.Buckman, *J. Phys. B* **33,** L309 (2000).
16. F.A Gianturco, R.R.Lucchese, N.Sanna, *J. Chem. Phys.* **102** 5743 (1995).
17. M.J.Brennan, D.T.Alle, P.Euripides, S.J.Buckman, M.J.Brunger, *J. Phys. B* **25,** *2669 (1992).*
18. W.M. Johnstone, W.R. Newell, *J. Phys. B* **24,** 473 (1991).
19. M.Allan, *J. Phys. B* **33,** L215 (2000).
20. W.C.Fon, K.A.Berrington, P.G.Burke, A.E.Kingston, *J. Phys. B* **22,** 3939 (1989).
21. B.Mielewska, G.C.King, M.Zubek, to be published.

ПРУЖНЕ І НЕПРУЖНЕ РОЗСІЮВАННЯ ЕЛЕКТРОНІВ АТОМАМИ І МОЛЕКУЛАМИ У ЗВОРОТНОМУ НАПРЯМІ

М.Зубек

Кафедра фізики електронних явищ, Технічний університет, 80-952 Гданськ, Польща

Повідомляються останні результати з досліджень розсіювання електронів атомами та молекулами на кути до 180^0. Обговорюються результати, одержані при кутах розсіювання від 120^0 до 180^0 для пружного і непружного розсіювання електронів з використанням методики магнітної зміни кута.