

## Relativistic low-energy elastic and momentum transfer cross sections for electron scattering from xenon

R P McEachran and A D Stauffer

Physics Department, York University, Toronto, Canada M3J 1P3

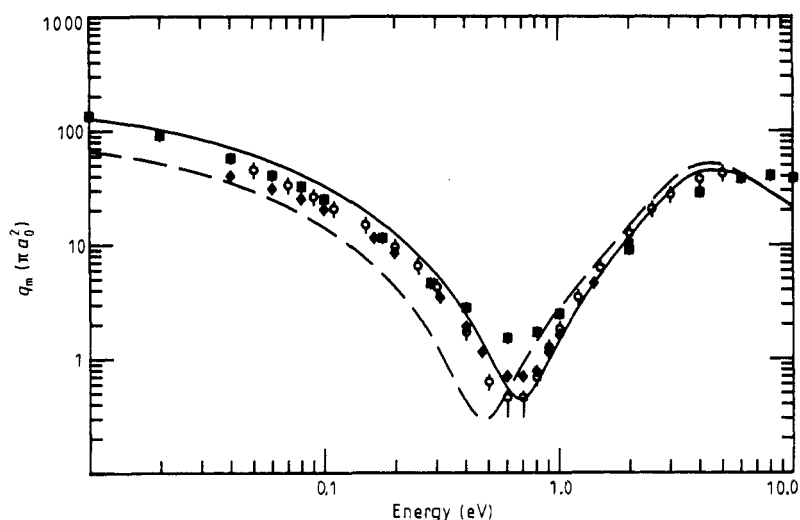
Received 28 January 1987

**Abstract.** We present results for the total elastic and momentum transfer cross sections for electron scattering from xenon in the energy range from 0 to 10 eV. These results were obtained by solving the Dirac equations including exchange and a non-relativistic polarisation potential. Very good agreement is obtained with recent experimental measurements and a comparison with our previous non-relativistic calculations confirms the importance of relativistic effects in xenon.

We have previously published results of a non-relativistic calculation for the elastic scattering of electrons from krypton and xenon at low energies (McEachran and Stauffer 1984). Recently, Koizumi *et al* (1986) have reported a new experimental determination of the momentum transfer cross section for these two gases in the energy range from threshold to 5 eV. In the case of krypton, there is quite good agreement between our previous calculations as well as with those of Fon *et al* (1984) and Sin Fai Lam (1982) and the new experimental results. However, for xenon there are systematic discrepancies, particularly in the position and magnitude of the Ramsauer minimum of the cross section. These discrepancies, which are attributed by Koizumi *et al* to relativistic effects, have prompted us to extend our recent relativistic calculations, in which we studied spin polarisation phenomena in electron–xenon scattering (McEachran and Stauffer 1986, hereafter referred to as I), to the study of the low-energy elastic and momentum transfer cross sections for this system.

In the present calculations we have solved the Dirac equations including exchange (equations (21*a*, *b*) of I) to which we have added our non-relativistic polarisation potential calculated via the polarised-orbital method (cf § 2.3 of I). These results do not differ significantly from those obtained using the relativistic form the Schrödinger equation, the method used in I. However, solving the Dirac equations directly avoids the approximations made in deriving the relativistic Schrödinger form and also eliminates the spurious resonances we occasionally encountered in solving the latter equation. In addition, the amount of computational effort required for these two methods is comparable so that there does not appear to be any good reason not to solve the Dirac equations directly.

In figure 1, we show our present results for the momentum transfer cross section for xenon along with our previous non-relativistic calculations (McEachran and Stauffer 1984) and the experimental results of Koizumi *et al* (1986), Frost and Phelps (1964) and Hoffman and Skarsgard (1969). The position of the Ramsauer minimum in our present calculations occurs at an energy approximately 0.2 eV higher than in our non-relativistic treatment and now agrees very well with the position of the minimum

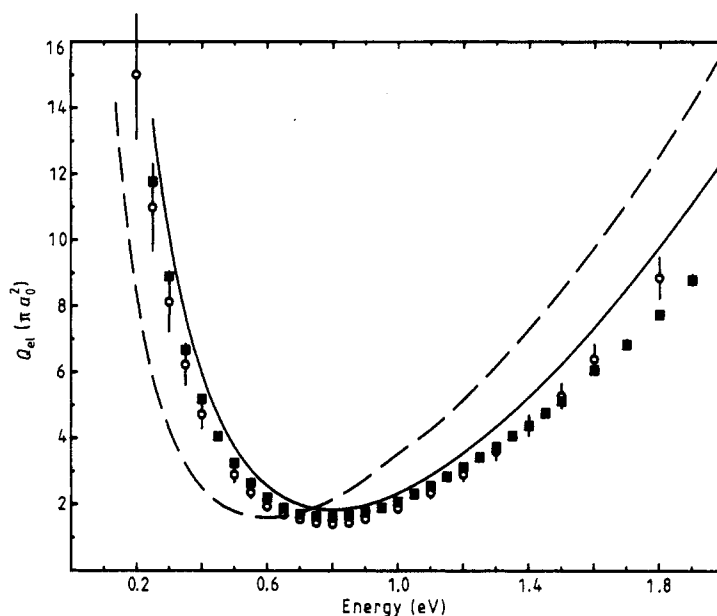


**Figure 1.** Momentum transfer cross section for electron scattering from xenon: (—), present relativistic calculations; (---), previous non-relativistic calculations (McEachran and Stauffer 1984); experimental results:  $\circ$ , Koizumi *et al* (1986);  $\blacksquare$ , Frost and Phelps (1964);  $\blacklozenge$ , Hoffmann and Skarsgard (1969).

shown in all three sets of experimental data. At and above the minimum, our present results agree very well in magnitude with the data of Koizumi *et al* and are distinctly lower than our non-relativistic values. Below the minimum, the relativistic values are considerably above the non-relativistic ones and the agreement with experiment is less good. However, Koizumi *et al* indicate that below 0.05 eV their method is not reliable and they have assumed the cross section values of Frost and Phelps for these energies. The other two sets of experimental data are comparable with Koizumi *et al* except in the region of the minimum where they are distinctly larger.

Sin Fai Lam (1982) has also performed calculations at a few energies in this range for the electron-xenon system using a relativistic form of the Schrödinger equation (see I for a detailed comparison with our previous work). Above the Ramsauer minimum his points agree fairly well with our relativistic calculation while below the minimum they fall approximately midway between our relativistic and non-relativistic results.

In figure 2 we show our present relativistic and previous non-relativistic results for the total elastic cross section for xenon over the energy range from 0 to 2 eV along with the experimental results of Jost *et al* (1983) and the recent measurements of Ferch *et al* (1987). We see here a similar improvement of our relativistic over our non-relativistic results as for the momentum transfer cross section. The shape of our relativistic cross section, including the position of the minimum, agrees very well with the data of Jost *et al* although we are slightly above the upper limit of the error bars on the experimental results over the energy range shown. The data of Ferch *et al* are in better agreement with our calculations at lower energies but above 1.4 eV they become systematically lower than our results and the measurements of Jost *et al*. The earlier measurements of Gus'kov *et al* (1978) are consistent with the other experimental data above the minimum but are distinctly lower below it and have a minimum at a lower energy. We present numerical values for the present calculation in table 1.



**Figure 2.** Total elastic cross section for electron scattering from xenon. The theoretical curves are as in figure 1; experimental results:  $\circ$ , Jost *et al* (1983);  $\blacksquare$ , Ferch *et al* (1987).

It is clear from these results that relativistic effects are important in the case of electron scattering from xenon and that their inclusion produces results that agree very well with recent experimental measurements. The remaining discrepancies between the theoretical and experimental results could well be accounted for by the inclusion of a polarisation potential which is determined within a relativistic framework.

**Table 1.** Total elastic and momentum transfer cross sections for xenon in  $\pi a_0^2$  as a function of energy.

eV	$Q_{el}$	$q_m$	eV	$Q_{el}$	$q_m$
0.01	133.514	127.122	0.80	1.831	0.605
0.02	108.312	100.616	0.90	1.976	0.953
0.03	91.180	82.883	1.00	2.338	1.438
0.04	78.736	70.169	1.20	3.546	2.738
0.05	68.963	60.283	1.50	6.227	5.374
0.07	54.612	45.992	2.00	12.499	11.500
0.09	44.537	36.160	2.50	20.741	19.587
0.11	37.052	28.998	3.00	30.435	28.746
0.15	26.758	19.438	4.00	48.714	43.212
0.20	18.788	12.391	5.00	57.422	43.737
0.25	13.649	8.108	6.00	57.907	40.466
0.30	10.196	5.409	7.00	55.407	34.202
0.40	5.985	2.429	8.00	52.447	28.830
0.50	3.739	1.089	9.00	49.775	24.560
0.60	2.556	0.552	10.00	47.536	21.180
0.70	1.980	0.440			

### Acknowledgments

We are grateful to Dr K Jost and Professor W Raith for providing us with detailed results of their experiments prior to publication. This research was supported in part by grants from the Natural Sciences and Engineering Research Council of Canada.

### References

- Ferch J, Simon F and Stakeljahn G 1987 *Proc. 15th Int. Conf. on Physics of Electronic and Atomic Collisions (Brighton)* Abstracts
- Fon W C, Berrington K A and Hibbert A 1984 *J. Phys. B: At. Mol. Phys.* **17** 3279-94
- Frost L S and Phelps V A 1964 *Phys. Rev.* **136** A1538-45
- Gus'kov Yu K, Savvov R V and Slobodyanyuk V A 1978 *Sov. Phys.-Tech. Phys.* **23** 167-71
- Hoffmann C R and Skarsgard H M 1969 *Phys. Rev.* **178** 168-75
- Jost K, Bisling P G F, Eschen E, Felsmann M and Walter L 1983 *Proc. 13th Int. Conf. on Physics of Electronic and Atomic Collisions (Berlin)* ed J Eichler *et al* (Amsterdam: North-Holland) Abstracts p 91
- Koizumi T, Shirakawa E and Ogawa I 1986 *J. Phys. B: At. Mol. Phys.* **19** 2331-42
- McEachran R P and Stauffer A D 1984 *J. Phys. B: At. Mol. Phys.* **17** 2507-18
- 1986 *J. Phys. B: At. Mol. Phys.* **19** 3523-38
- Sin Fai Lam L T 1982 *J. Phys. B: At. Mol. Phys.* **15** 119-42