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LETTER TO THE EDITOR

# Elastic scattering of fast electrons and positrons by argon†

C J Joachain‡, K H Winters‡ and F W Byron Jr§

‡ Physique Théorique, Faculté des Sciences, Université Libre de Bruxelles, Brussels, Belgium
§ Department of Physics and Astronomy, University of Massachusetts, Amherst, Massachusetts 01002, USA

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**Abstract.** We use an *ab initio* optical model theory to analyse the elastic scattering of electrons and positrons by argon in the energy region 100 eV–1 keV. Our calculations are compared with recent absolute measurements of differential cross sections for electron scattering. Total cross sections for electron and positron collisions with argon are also discussed.

Recent absolute measurements of differential cross sections for the elastic scattering of fast electrons by noble gases (see eg Jansen *et al* 1974, 1975) are of considerable interest as they provide a good test of theoretical calculations. Moreover, total cross sections for both electron and positron scattering by noble gases have been obtained.

For the relatively simple case of scattering by helium, several theoretical methods have been developed with great success, in particular the second-order potential approach (Winters *et al* 1973, 1974), the eikonal-Born series theory (Byron and Joachain 1973a, b, 1975a) and the *ab initio* optical model theory of Byron and Joachain (1974a, b, 1975b). This latter approach is particularly useful when dealing with complex target atoms, and has already been successfully generalized to the case of neon (Byron and Joachain 1974b, 1975b). In this letter we extend further this *ab initio* optical model to analyse the elastic scattering of fast electrons and positrons by argon, a case for which few theoretical calculations are available (Walker 1971, Thompson 1971, Pindzola and Kelly 1974, Khare and Shobha 1974).

Our treatment uses the basic ideas of the eikonal-Born series method within the framework of the optical potential formalism. The direct part of the exact optical potential, $V^{\mathrm{d}}_{\mathrm{opt}}$, is first expanded through second-order in the full projectile–target interaction $V$ giving

$$V^{\mathrm{d}}_{\mathrm{opt}} \simeq V^{(1)} + V^{(2)}. \tag{1}$$

Here $V^{(1)} = \langle 0|V|0\rangle$ is the static potential, $|0\rangle$ being the ground state of the target. This potential is dominant at short distances and therefore strongly influences the large angle scattering. On the other hand, since $V^{(1)}$ is real and of short range, a description of the scattering in terms of this potential alone (Fink and Yates 1970) is inadequate at small momentum transfers. This conclusion is unaltered by the inclusion of exchange effects which, for incident electrons, leads to the so-called static-exchange approximation.

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The second-order part $V^{(2)}$ of the direct optical potential is obtained in the following way. First, an average target excitation energy $\Delta$ is used to perform the sum over intermediate target states by closure (Joachain and Mittleman 1971, Bransden and Coleman 1972). Using properties of the Born and Glauber series, we then approximate the resulting complex *non-local* potential by a complex local one of the form

$$V^{(2)} = V_{\text{pol}} + \mathrm{i}V_{\text{abs}} \tag{2}$$

where $V_{\text{pol}}$ and $V_{\text{abs}}$ account respectively for polarization and absorption effects and are given explicitly elsewhere (Byron and Joachain 1974a, 1975b).

Finally, exchange effects, occurring for incident electrons, are taken into account by adding to $V^{\text{d}}_{\text{opt}}$ a pseudopotential $V^{\text{ex}}_{\text{opt}}$ (Mittleman and Watson 1960). Both $V^{\text{d}}_{\text{opt}}$ and $V^{\text{ex}}_{\text{opt}}$ were determined by using the Hartree–Fock wavefunction of Clementi (1965) to describe the target ground state $|0\rangle$.

Having determined the optical potential, we then use the partial-wave method and solve numerically the radial Schrödinger equations. As an example, figures 1(*a*) and (*b*) show our differential cross section for elastic electron–argon scattering at an incident electron energy of 500 eV, for small and large angles respectively. We note that even at this rather high energy the first Born approximation is very inaccurate. We also remark from figure 1(*a*) that our calculations are in excellent agreement with the experimental data of Bromberg (1974), DuBois and Rudd (1974) and Jansen *et al* (1974, 1975). This agreement at small angles persists down to lower energies. On the other hand, the

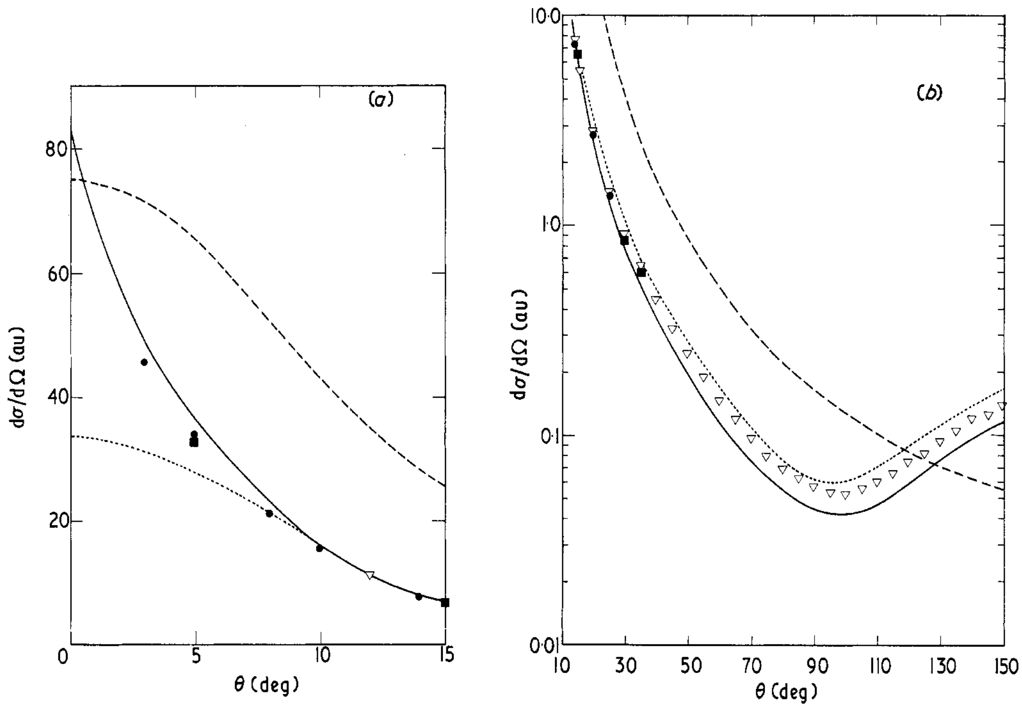


**Figure 1.** Differential cross sections at (*a*) small and (*b*) large angles for the elastic scattering of 500 eV electrons from argon. Full curve: present results; broken curve: first Born approximation; dotted curve: static approximation (partial-wave treatment of the static potential $\langle 0|V|0\rangle$). ●: Bromberg (1974); ■: Jansen *et al* (1975); ▽: DuBois and Rudd (1974).

static approximation (Fink and Yates 1970) fails at small angles, as expected. It is also worth noting that *both* polarization and absorption effects are important in this angular range.

Regarding the large-angle situation, we see that the static results agree with the experimental data as well as our more elaborate calculations. This is due to delicate cancellations between absorption and exchange effects. The latter would of course not be present for *positron* scattering so that we might expect the static model to be less accurate for that case. Moreover, our use of eikonal methods to obtain $V_{abs}$ leads to an overestimate of absorption effects at large angles and for heavy atoms, since the semi-classical condition $ka \gg 1$ is only fulfilled for the innermost shell at rather high energies. Thus at lower energies our theoretical values underestimate the large-angle cross sections.

Finally, we present in tables 1 and 2 our total cross sections, respectively for electron and positron scattering by argon. Our electron results are seen to be in fair agreement with the experimental data of Jansen *et al* (1974, 1975) at energies above 200 eV, while the earlier results of Normand (1930) fall systematically on the low side of our calculations. The recent semi-empirical total cross sections of de Heer and Jansen (1975) are in better agreement with our results, particularly at high energies. Regarding positron–argon scattering, the preliminary measurements of Coleman *et al* (1975) agree well with our calculations at 100 eV, but are in serious disagreement at higher energies. Further positron data in this energy domain are clearly desirable.

**Table 1.** Total cross sections (in units of $a_0^2$) for electron–argon scattering.

| | | Experimental values | | |
|---|---|---|---|---|
| Energy (eV) | Present theory | Normand (1930) | Jansen *et al* (1975) | de Heer and Jansen (1975) |
| 100 | 33·4 | 22·5 | 18·8 | 25·5 |
| 200 | 23·8 | 16·4 | — | 20·2 |
| 300 | 19·1 | 12·8 | 14·1 | 16·8 |
| 400 | 16·2 | 10·8 | — | 14·4 |
| 500 | 14·2 | — | 11·0 | 12·6 |
| 800 | 10·5 | — | — | — |
| 1000 | 9·04 | — | 6·8 | 8·01 |

**Table 2.** Total cross sections (units of $a_0^2$) for positron–argon scattering.

| Energy (eV) | Present theory | Experiment Coleman *et al* (1975) |
|---|---|---|
| 100 | 22·8 | 24·5 |
| 200 | 18·5 | 13·2 |
| 300 | 15·7 | 9·10 |
| 400 | 13·8 | 6·60 |
| 500 | 12·3 | — |

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