J. Phys. B: At. Mol. Opt. Phys. 26 (1993) 2733–2739. Printed in the UK

Calculation of total cross sections for electron and positron scattering on sodium and potassium

I E McCarthy, K Ratnavelu† and Y Zhou
Electronic Structure of Materials Centre, School of Physical Sciences, Flinders University, GPO Box 2100, Adelaide 5001, Australia

Received 8 March 1993, in final form 28 May 1993

Abstract. Total cross sections for electron and positron scattering on sodium and potassium are calculated at various energies and compared with experiment. The method used is the coupled-channels-optical method with the equivalent-local polarization potential, which takes all channels into account. For electrons the calculations are checked by comparison with coupled-channels-optical calculations using a detailed polarization potential that makes only one approximation, that of weak coupling in the ionization space. The polarization potential for positrons includes effects of ionization and positronium formation.

1. Introduction

For calculating the collisions of electrons or positrons with atoms we now have methods that take all channels into account. The total cross section is an important check on the overall validity of a method.

The coupled-channels-optical (CCO) calculation (McCarthy and Stelbovics 1983, Bray *et al* 1989, 1991a) has had much success for electron–hydrogen collisions at all energies and remarkable success for electron–sodium collisions (Bray and McCarthy 1993) for which it gives detailed agreement with experiment for differential cross sections, magnetic substate parameters and spin-dependent data. The most detailed version of this calculation solves the coupled integral equations for a set of discrete channels (P space), whose effects on the low-lying channels under discussion have converged. The target continuum is represented by adding an *ab initio* polarization potential to the coupling potential. The only approximation made is the neglect of coupling of channels within the continuum space (Q space). A simpler version of the polarization potential makes an equivalent-local approximation for the matrix elements of the polarization potential (McCarthy and Weigold 1991). This version also reproduces the most critical effect of the polarization potential for sodium, the reversal of the sign of the 3p asymmetry at some energies (McCarthy *et al* 1991).

Here we apply the CCO method with the equivalent-local polarization potential to the total cross section for electron and positron collisions on sodium and potassium. The results are compared with recent measurements by Kwan *et al* (1991).

There have been no earlier calculations of these reactions that treat all channels, apart from those employing the CCO method. For electrons Msezane (1988) has coupled the six lowest-lying channels of sodium and for positrons Ward *et al* (1989) have coupled the five lowest-lying channels for both targets. For the latter calculation the authors believe that the effect of the continuum on the total cross section is negligible. References to other calculations are given by Kwan *et al* (1991).

† Permanent address: Department of Mathematics, University of Malaya, 59100 Kuala Lumpur, Malaysia.

0953-4075/93/162733+07$07.50

2. Outline of the method

The coupled-channels-optical method consists of the solution of a discrete set of coupled Lippmann–Schwinger integral equations for the T-matrix elements (McCarthy and Stelbovics 1983).

$$\langle k'i|T|0k_0\rangle = \langle k'i|V^{(Q)}|0k_0\rangle + \sum_{j\in P}\int \mathrm{d}^3q\langle k'i|V^{(Q)}|jq\rangle \times \frac{1}{E^{(+)} - \epsilon_j - \frac{1}{2}q^2}\langle qj|T|0k_0\rangle \qquad i \in P \tag{1}$$

where the target states $|i\rangle$, $|j\rangle$ are defined by the target Hamiltonian H_T.

$$\left[\epsilon_j - H_T\right]|j\rangle = 0. \tag{2}$$

The matrix elements of the optical potential are

$$\langle k'i|V^{(Q)}|jk\rangle = \langle k'i|V|jk\rangle + \sum_n \langle k'i|V|Q\Psi_n^{(-)}\rangle \frac{1}{E^{(+)} - E_n}\langle \Psi_n^{(-)}Q|V|jk\rangle \tag{3}$$

where V is the electron target potential and Q is the projection operator for Q space

$$Q = \sum_{n\in Q}|\Psi_n^{(-)}\rangle\langle\Psi_n^{(-)}|. \tag{4}$$

For the collision states $|\Psi_n^{(-)}\rangle$ we use a discrete notation for the one- or two-body continuum. In the case of a positron projectile the two-body continuum includes both ionization and positronium-formation channels. The superscript $(\pm)$ notation indicates outgoing or ingoing spherical-wave boundary conditions respectively.

The collision is considered as the three-body problem of an electron or positron projectile, a target electron and an inert closed-shell ion. The electron–ion potential is the frozen-core Hartree–Fock potential.

The second term of (3) is the complex, non-local polarization potential, which depends on the full solution of the problem for collision states with entrance channel $n \in Q$. These must of course be approximated. The partial-wave polarization potential (PWP) using symmetric P and Q operators has been discussed by Bray *et al* (1991a, b) for electrons. Continuum states are separated in the state vectors of the two electrons. The state vector of the target electron is calculated in the frozen-core Hartree–Fock potential. The projectile is represented by a plane wave orthogonalized to P space.

The matrix elements of the equivalent-local polarization potential (ELP) are calculated by multidimensional integration. Sufficient computational speed is achieved only by making analytic approximations for the integrand. In practice we need only continuum states in the polarization potential, since we treat P space to convergence. For ionization we approximate the slow electron or positron state by a Coulomb wave orthogonalized to the appropriate target state and the faster particle by a plane wave. For positronium formation we use positronium states with the centre-of-mass motion represented by a plane wave. In addition we make equivalent-local approximations for both direct and exchange matrix elements (Lower *et al* 1987).

Satisfactory convergence is achieved for the ELP calculation by including the lowest-lying eight channels in P space. For sodium they are 3, 4, 5s; 3, 4, 5p; 3, 4d. Polarization potentials are calculated only for the couplings 3s–3s, 3s–3p and 3p–3p. Potassium calculations are similar with principal quantum numbers increased by 1. The PWP calculation has stricter convergence criteria. P space consists of the lowest-lying 15 channels for sodium and all couplings of the lowest-lying six have polarization potentials.

Table 1. Total cross sections (10^{-16} cm^2) for electron and positron scattering on sodium. Expt, experimental data of Kwan *et al* (1991); ELP, present calculation using equivalent local polarization potential; PWP, partial-wave polarization potential (Bray *et al* 1991b).

E (eV)	Expt	ELP	PWP
Electrons			
4.1	67.1±14.1	—	89.5
5.9	66.5±14.0	—	78.6
10.8	55.9±11.7	72.3	61.1
20.7	43.3±9.1	54.1	49.1
30.7	32.6±6.8	43.5	40.5
40.8	30.0±6.3	36.5	34.6
50.8	26.2±5.5	31.2	31.6
60.9	22.9±4.8	27.5	28.8
76.1	22.0±4.6	23.3	24.6
Positrons			
17.7	52.1±10.9	55.3	—
27.7	40.8±8.6	45.7	—
37.6	33.5±7.0	38.7	—
48.3	28.8±6.0	32.0	—
57.9	22.0±4.6	27.3	—
73.3	19.1±4.0	22.3	—
98.3	18.3±3.8	18.6	—

Table 2. Total cross sections (10^{-16} cm^2) for electron and positron scattering on potassium. Expt, experimental data of Kwan *et al* (1991); ELP, present calculation using equivalent local polarization potential; PWP, partial-wave polarization potential (Bray *et al* 1993).

E (eV)	Expt	ELP	PWP
Electrons			
4.4	90.3±19.0	—	142.8
6.2	89.6±18.8	—	119.0
11.0	77.7±16.3	116.2	101.7
21.2	65.1±13.7	72.3	78.7
31.3	51.6±10.8	54.7	64.1
41.4	43.9±9.2	48.8	54.0
51.4	42.1±8.8	46.5	47.6
76.8	37.5±7.9	41.3	35.3
101.9	31.5±6.6	36.2	28.3
Positrons			
7.9	106.1±22.3	107.6	—
18.0	75.7±15.9	86.4	—
28.1	59.1±12.4	66.8	—
38.2	47.9±10.1	53.9	—
48.2	42.1±8.8	46.1	—
73.5	34.7±7.3	35.3	—
98.5	30.1±6.3	29.1	—

3. Comparison with experiment

Table 1 compares the total cross sections for sodium calculated by the CCO-ELP method with the experimental data of Kwan *et al* (1991). In order to check approximations the CCO-PWP cross sections, calculated by the method of Bray and McCarthy (1992) are included for electrons. In both calculations Q space includes only the two-particle

continuum, i.e. ionization for electrons and both ionization and positronium formation for positrons. The ELP calculation of the polarization potential gives larger cross sections than experiment for electrons at the lower energies. It is considered to be unrealistic below 10 eV, where the plane-wave and equivalent-local approximations are invalid. The PWP calculation, as expected, is much better at the lower energies and usually gives a cross section within the experimental error, while tending again to overestimate. For positrons the ELP calculation achieves cross sections within experimental error. Table 2 gives the corresponding comparison for potassium. For the ELP calculation the eight channels of P space have principal quantum numbers one higher than for sodium. Again P space is included to convergence in the PWP calculation. In this case this involves the lowest 17 channels (Bray *et al* 1993). For electrons both ELP and PWP again tend to overestimate the total cross section at energies below about 10 eV, but both agree quite well at higher energies. For positrons ELP again agrees within experimental error.

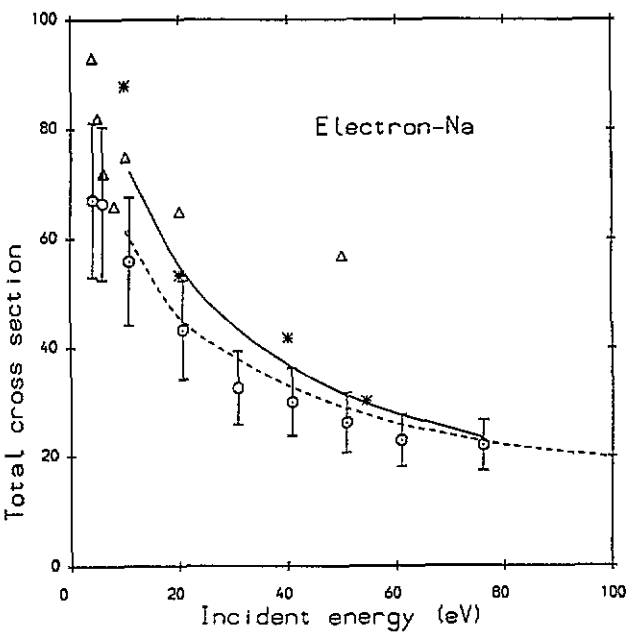

Figure 1. Total cross section (units 10^{-16} cm^2) for electron scattering from sodium. Open circles, Kwan *et al* (1991); asterisks, Srivastava and Vušković (1980); triangles, Kasdan *et al* (1973); full curve, present eight-state CCO-ELP; broken curve, six-state CC (Msezane 1988).

The comparison of the eight-channel CCO-ELP calculation with experimental data and smaller coupled-channels calculations is summarized in figures 1–4.

4. Discussion and conclusions

Total cross sections provide an important check on the treatment of channels that are not explicitly coupled in a reaction calculation that takes all channels into account. The CCO method with both the equivalent-local and partial-wave calculations of the polarization potential obeys this check for electrons on sodium and potassium at the relatively high

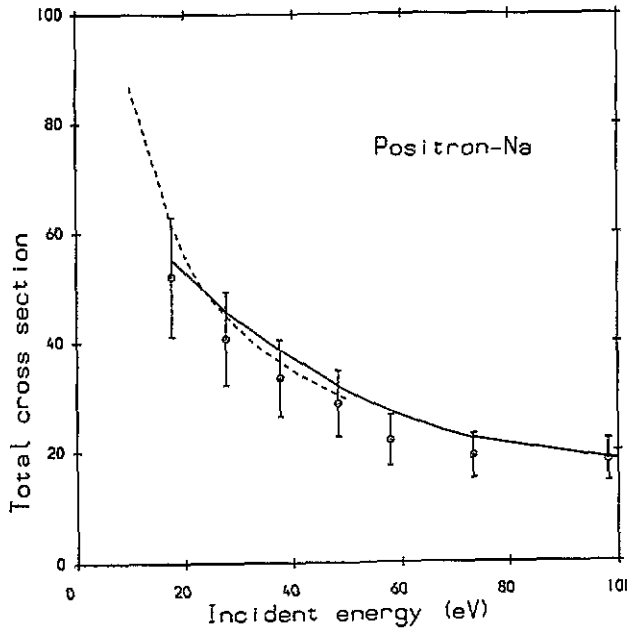

Figure 2. Total cross section (units 10^{-16} cm^2) for positron scattering from sodium. Open circles, Kwan *et al* (1991). Full curve, present eight-state CCO-ELP; broken curve, five-state CC (Ward *et al* 1989).

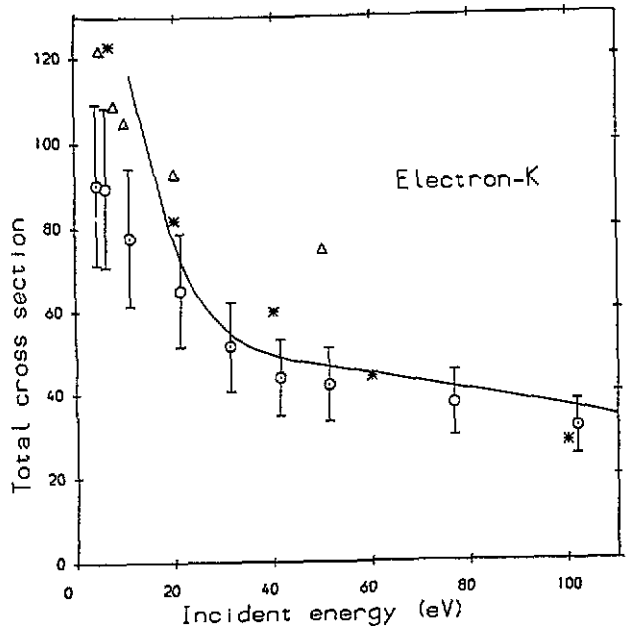

Figure 3. Total cross section (units 10^{-16} cm^2) for electron scattering from potassium. Open circles, Kwan *et al* (1991); asterisks, Vušković and Srivastava (1980); triangles, Kasdan *et al* (1973). Full curve, present eight-state CCO-ELP.

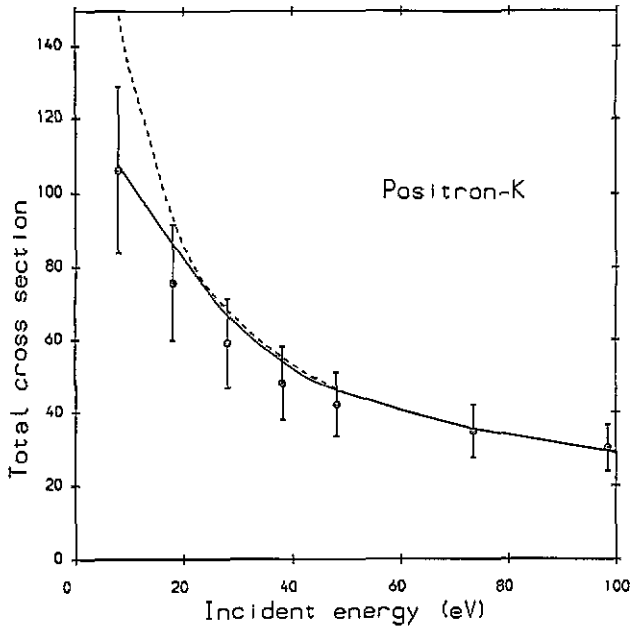

Figure 4. Total cross section (units 10^{-16} cm^2) for positron scattering from potassium. Open circles, Kwan *et al* (1991); full curve, present eight-state CCO-ELP; broken curve, five-state CC (Ward *et al* 1989).

energies, above about 20 eV, where the approximations made for ELP are expected to be valid. The equivalent-local approximations are made for computational feasibility. The PWP calculation does not make these approximations. Its validity extends to lower energies.

Although the total cross section supplies a necessary test of validity, it is not sensitive. For example in the electron–sodium case at 50.8 eV the contribution to the total cross section from excitation of the eight explicitly-coupled channels is 29.6×10^{-16} cm^2 compared with a total of 31.2×10^{-16} cm^2 in the ELP calculation. The effect of the continuum on electron differential cross sections for sodium and potassium is also quite small (Bray *et al* 1991b, 1993). Its effect is critical in accounting successfully for elastic and inelastic asymmetries (Bray and McCarthy 1993, McCarthy *et al* 1991) in both the PWP and ELP approximations. The CCO-PWP method is successful for all data at all energies in the case of electron collisions with sodium and potassium. The tendency of this method to somewhat overestimate the present total cross sections at very low energy does not affect its validity for differential cross sections and asymmetries. The CCO-ELP method overestimates total cross sections at very low energies.

The CCO-ELP method accounts successfully for the present positron total cross sections. Again it is insensitive to the continuum. At 48.3 eV for sodium the eight explicitly-coupled channels account for 31.5×10^{-16} cm^2 out of a total of 32.0×10^{-16} cm^2.

Recent experimental data (Parikh *et al* 1993) at energies below 10 eV will provide a further test of CCO methods.

Acknowledgments

We thank Dr I Bray for help with the CCO-PWP calculations. We acknowledge support from the Australian Research Council.

References

Bray I, Fursa D and McCarthy I E 1993 to be published
Bray I, Konovalov D A and McCarthy I E 1991a *Phys. Rev.* A **44** 5586
—— 1991b *Phys. Rev.* A **44** 7179
Bray I and McCarthy I E 1993 *Phys. Rev.* A **47** 317
Bray I, McCarthy I E, Mitroy J and Ratnavelu K 1989 *Phys. Rev.* A **39** 4998
Kasdan A, Miller T M and Bederson B 1973 *Phys. Rev.* A **8** 1562
Kwan C K, Kauppila W E, Lukaszew R A, Parikh S P, Stein T S, Wan Y J and Dababneh M S 1991 *Phys. Rev.* A **44** 1620
Lower J, McCarthy I E and Weigold E 1987 *J. Phys. B: At. Mol. Phys.* **20** 4571
McCarthy I E, Mitroy J and Nicholson R JF 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** L449
McCarthy I E and Stelbovics A T 1983 *Phys. Rev.* A **28** 2693
McCarthy I E and Weigold E 1991 *Adv. At. Mol. Opt. Phys.* **27** 165
Msezane A Z 1988 *Phys. Rev.* A **37** 1787
Parikh S P, Kauppila W E, Kwan C K, Lukaszew R A, Przybyla D, Stein T S and Zhou S 1993 *Phys. Rev.* A **47** 1535
Srivastava S K and Vušković L 1980 *J. Phys. B: At. Mol. Phys.* **13** 2633
Vušković L and Srivastava S K 1980 *J. Phys. B: At. Mol. Phys.* **13** 4849
Ward S J, Horbatsch M, McEachran R P and Stauffer A D 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 1845