# ELECTRONIC STRUCTURE OF MATERIALS CENTRE

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## 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 polarisation potential, which takes all channels into account. For electrons the calculations are checked by comparison with coupled-channels-optical calculations using a detailed polarisation potential that makes only one approximation, that of weak coupling in the ionisation space. The polarisation potential for positrons includes effects of ionisation and positronium formation.

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## 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, McCarthy, Mitroy and Ratnavelu 1989; Bray, Konovalov and McCarthy 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 polarisation 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 polarisation potential makes an equivalent-local approximation for the matrix elements of the polarisation potential (McCarthy and Weigold 1991). This version also reproduces the most critical effect of the polarisation potential for sodium, the reversal of the sign of the 3p asymmetry at some energies (McCarthy, Mitroy and Nicholson 1991).

Here we apply the CCO method with the equivalent-local polarisation 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).

## 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).

$$\langle \mathbf{k}'i|T|0\mathbf{k}_0\rangle = \langle \mathbf{k}'i|V^{(Q)}|0\mathbf{k}_0\rangle + \sum_{j\in P}\int d^3q \langle \mathbf{k}'i|V^{(Q)}|j\,\mathbf{q}\rangle \times \frac{1}{E^{(+)} - \epsilon_j - \frac{1}{2}q^2}\langle \mathbf{q}j|T|0\mathbf{k}_0\rangle, \quad i \in P, \tag{1}$$

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

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

The matrix elements of the optical potential are

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

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

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

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 ionisation 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, nonlocal polarisation 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 polarisation 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 orthogonalised to $P$ space.

The matrix elements of the equivalent-local polarisation 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 polarisation potential, since we treat $P$ space to convergence. For ionisation we approximate the slow electron or positron state by a Coulomb wave orthogonalised 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, McCarthy and Weigold 1987).

Satisfactory convergence is achieved for the ELP calculation by including the lowest-lying 8 channels in $P$ space. For sodium they are 3,4,5s; 3,4,5p; 3,4d. Polarisation 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 6 have polarisation potentials.

## 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 the approximations the CCO-PWP cross sections of Bray and McCarthy (1992) are included for electrons. In both calculations $Q$ space includes only the two-particle continuum, i.e. ionisation for electrons and both ionisation and positronium formation for positrons. The ELP calculation of the polarisation potential gives larger cross

sections than experiment for electrons at the lower energies. It is considered to be unrealistic below 10eV, 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 8 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, Fursa and McCarthy 1993). For electrons both ELP and PWP again tend to overestimate the total cross section at energies below about 10eV, but both agree quite well at higher energies. For positrons ELP again agrees within experimental error.

## 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 polarisation potential obeys this check for electrons on sodium and potassium at the relatively-high energies, above about 20eV, 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 50.8eV the contribution to the total cross section from excitation of the 8 explicitly-coupled channels is $29.6 \times 10^{-16}\text{cm}^2$ compared with a total of $31.2 \times 10^{-16}\text{cm}^2$ 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, Bray *et al.* 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 48.3eV the 8 explicitly-coupled channels account for $32.2 \times 10^{-16}\text{cm}^2$ out of a total of $33.3 \times 10^{-16}\text{cm}^2$.

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

| E(eV) | EXP | 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 | — | 34.6 |
| 50.8 | 26.2± 5.5 | 31.2 | 31.6 |
| 60.9 | 22.9± 4.8 | 27.6 | 28.8 |
| 76.1 | 22.0± 4.6 | 23.3 | 24.6 |
| **Positrons** | | | |
| 17.7 | 52.1±10.9 | 51.9 | — |
| 27.7 | 40.8± 8.6 | 43.9 | — |
| 37.6 | 33.5± 7.0 | 39.3 | — |
| 48.3 | 28.8± 6.0 | 33.3 | — |
| 57.9 | 22.0± 4.6 | 27.3 | — |
| 73.3 | 19.1± 4.0 | 22.3 | — |
| 98.3 | 18.3± 3.8 | 20.9 | — |

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

| E(eV) | EXP | 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 | 75.8 | — |
| 28.1 | 59.1±12.4 | 66.8 | — |
| 38.2 | 47.9±10.1 | 56.6 | — |
| 48.2 | 42.1± 8.8 | 46.1 | — |
| 73.5 | 34.7± 7.3 | 35.3 | — |
| 98.5 | 30.1± 6.3 | 33.5 | — |