Positron scattering from noble gases

D. V. Fursa and I. Bray
ARC Centre for Antimatter-Matter Studies,
Curtin University, GPO Box U1987, Perth, WA 6845, Australia
E-mail: d.fursa@curtin.edu.au

Abstract. We have extended the nonrelativistic convergent close-coupling (CCC) method to the calculation of positron scattering from noble gases within the single-centre approximation. Good agreement is found with the available measurements of total cross sections and elastic differential cross sections for Ne, Ar, Kr and Xe.

1. Introduction
Theoretical description of positron-scattering on atoms and molecules is somewhat similar to that of electron scattering, and superficially might even look simpler as complications associated with the Pauli exclusion principle do not apply. As with electrons, positron collisions lead to elastic scattering, target excitation and ionization. In place of the exchange channels, positron scattering has channels known as positronium (Ps) formation, where the incident positron captures an atomic electron to form a positronium atom. Account of the positronium formation channels represents a major difficulty in the theoretical treatment of positron collisions with atoms and molecules.

Interaction of positrons with atoms [1] includes the short ranged repulsion from the atomic nucleus while at the larger distances the polarization of the electron cloud by the incident positron leads to an attractive polarization potential, \( V(r) = -\alpha_d e^2 / 2 r^4 \), where \( \alpha_d \) is the dipole polarizability of the atom. At low energies, virtual Ps formation leads to an effective attractive potential between the positron and the atom. An adequate account of these interactions is important for an accurate description of positron-atom scattering, requiring a two-centre (atom and Ps) approach to the problem.

McAlinden and Walters [2] performed two-centre close-coupling calculations in the (truncated) coupled-static approximation, with results presented for positronium formation and elastic scattering cross sections. To date it is the only two-centre close coupling calculation applied to the heavier noble gases. Establishing convergence in such calculations with differing bases is notoriously difficult. Several theoretical methods applied to positron scattering from noble gases are variants of the single channel optical potential method (see [3, 4, 5] for detailed discussion). These methods model interaction of positrons with atoms using an optical potential whose real part is a sum of static plus polarization terms, while the imaginary part, i.e. the absorption potential, is constructed to account for excitation and ionization channels. No account of positronium formation channels is done in these calculations. Results of such calculations vary considerably depending on the accuracy of the polarization potential.

Here we present the results of a single-centre convergent close-coupling (CCC) method as applied to positron-noble gas scattering. While this lacks explicit Ps-formation, the positive-
energy pseudostates take into account virtual Ps-formation at energies below the Ps-formation threshold, and at energies above the ionization threshold they represent both ionization and Ps-formation channels. Our results for the grand total cross sections and elastic differential cross sections are compared with the measurements for for Ne, Ar, Kr and Xe.

2. Theoretical method
We use the nonrelativistic approximation to describe the target structure of noble gases. Taking Ne as an example, the wave functions are described in a model of six $p$-electrons above an inert Hartree-Fock core with only one-electron excitations from the $p^6$ shell allowed. Inert core orbitals ($1s^22s^2$) and the “frozen” $2p$ orbital are obtained from a self-consistent Hartree-Fock calculation for the ground state of the Ne$^+$ ion. Next, we conduct configuration interaction calculations by diagonalizing the target Hamiltonian in the basis of all possible $2p^5nl$ configurations,

$$\psi_a = A \sum_m \xi_m(x_N) \psi_c^{+}(p^5).$$

Here $A$ is antisymmetrization operator, $\psi_c$ represents the $p^5$ frozen-core wave function. The active electron $\phi_{nl}$ is represented by the square-integrable Laguerre basis $\xi_{nl}$. This approach allows us to model the bound and the continuous spectra of noble gases, and is somewhat similar to the frozen-core model we have successfully utilized for electron-helium scattering [6]. The frozen-core wave function has angular momentum $l_c = 1$ and spin $s_c = 1/2$, and when coupled with the active electron wave function $\phi_{nl}$, leads to the target state wave function $\psi_a$ with spin $s_a = 0, 1$ and angular momentum $l_a = l, l \pm 1$. For scattering from the ground state of noble gases ($s_a = 0, l_a = 0$) only singlet states ($s_a = 0$) will be excited.

In the Table we present comparison of the resultant ionization energies and the static dipole polarizabilities with the experimental values. We see that the agreement with experiment for Ne, Ar, Kr, and Xe is of the same quality as for He (also frozen-core model). We note that for noble gases a major part of the static dipole polarizability comes from the target continuum.

| Ionization energy (eV) | Static dipole polarizability (a.u.) |
|------------------------|----------------------------------|
| CCC                    | experiment [7]                   |
| Ne 20.57               | 3.0                              |
| Ar 14.95               | 13.8                             |
| Kr 13.38               | 21.3                             |
| Xe 11.73               | 35.4                             |
| He 23.74               | 1.53                             |

The single-centre CCC method solves the Schrödinger equation by expanding the total scattering wave function in a large set of target states

$$\Psi = \sum a F_a(r_p)\psi_a(x_1, ..., x_N),$$

where $F_a$ is a positron channel function. This leads to coupled Lippmann-Schwinger equations for the T-matrix,

$$T_{f_1}(k_f, k_i) = V_{f_1}(k_f, k_i) + \sum_{n=1}^{N} \int d^3k V_{fn}(k_f, k) T_{nl}(k, k_i) \frac{V_{ln}(k_f, k) T_{ni}(k, k_i)}{E + i0 - \epsilon_k - \epsilon_n}.$$
This equation is solved via standard methods [6], with the $V$-matrix elements in the present case given by Fursa and Bray [9]. The scattering amplitudes and cross sections are generated for each transition directly from the partial wave expansion of the $T$-matrix. The grand total cross section is obtained by summation of cross sections for all negative- and positive-energy nstates.

The positronium formation channels are not accounted for explicitly, but are included indirectly via close-coupling expansions that include a large number of positive-energy pseudostates of high orbital angular momentum. For incident positron energies above the target atom ionization threshold the total ionization cross section obtained in the CCC method provides an accurate estimate of the sum of direct ionization and positronium formation. In the low energy region where positronium formation channels are closed the CCC method can again provide an accurate estimate of elastic scattering cross sections. In this case virtual Ps-formation channels, which play a vital role in the scattering, are also taken into account. The incident energy region between the Ps-formation threshold and the ionization threshold are problematic. At these energies the positronium formation channels are open, but the positive energy pseudostates that model the break-up are closed. As a result a lack of convergence is found on this small energy range.

![Figure 1](image_url)

**Figure 1.** Grand total cross section for positron-helium scattering. Single-centre scCCC calculations performed in the frozen-core (FC) and multi-core (MC) models are compared with corresponding two-centre CCC calculations [10]. Experiment is due to Caradonna et al. [11].

We can estimate how much the accuracy of our structure model will affect the scattering results by comparing results for positron-helium scattering obtained in the frozen-core model with those obtained in the more accurate multi-core model of helium. Figure 1 presents this comparison for the grand total cross section calculated in the single-centre and two-centre methods [10]. We note the very good agreement between single- and two-centre calculations performed in the same structure model. This validates the single-centre CCC approach, which currently is the only one implemented for the heavier noble gases. We observe a reduction of the cross sections as the helium structure improves from the frozen-core to multi-core models. Such
A reduction of the cross sections can be understood by noting that the static dipole polarizability of helium calculated in the frozen-core model is larger than the experimental value (see Table), which leads to a somewhat too strong attractive polarization potential, and consequently to overestimation of the cross sections. A simple way to reduce the static dipole polarizability of the target atom is to modify the dipole term of the Coulomb potential (both electron-electron and positron-electron) with a model polarization potential [12]

\[ V = -\frac{\alpha_d}{r_1^3 r_2^3} (r_1, r_2) \sqrt{(1 - e^{-r_1/\rho})^6(1 - e^{-r_2/\rho})^6}, \]  

Here \( \alpha_d \) is the static dipole polarizability of the atom and parameter \( \rho \) is chosen in such a way as to fit the calculated static dipole polarizability to the experimental value. We have adopted this approach in all calculations presented here.

Finally, we note that Xe is a sufficiently heavy atom for which a relativistic approach is preferable. This is particularly important for excited states of Xe. However, for elastic scattering, and aggregate observables such as the total cross section, the use of a nonrelativistic CCC approach is likely to be sufficiently accurate.

3. Results and discussion

We start with the presentation of the differential cross sections for positron scattering from Xe at 1 and 15 eV. Figure 2 compares the CCC results with absolute experimental cross sections [5], the theoretical results of Sin Fail Lam [13] and the relativistic optical potential (ROP) calculations of McEachran [5]. At 1 eV the results of Sin Fail Lam [13] have been obtained with a simplified form of the polarization potential and significantly underestimate the cross section, while CCC and ROP methods are in very good agreement with experiment. The CCC and ROP results are in good agreement with each other except for the forward scattering angles. This can be attributed to virtual positronium formation that is accounted for in the CCC method but not in ROP method. The large difference between ROP calculations and those of and Sin Fail Lam [13] indicates the importance of an accurate treatment of target polarization. At larger energies, above the ionization threshold the CCC and ROP calculations predict very different cross section values at forward scattering, with the CCC results being in good agreement with experiment. The difference between the CCC and ROP results is due to the open positronium formation channels. These are not represented in the ROP method, while the CCC method takes into account coupling to the positronium formation channels via close coupling expansions with large target space orbital angular momentum. Account of such additional reaction channels leads to the enhancement of forward scattering.

Figures 3-6 present grand total cross sections for positron scattering from Ne, Ar, Kr, and Xe, respectively. Cross sections have similar features for all considered atoms. It has a plateau at larger incident positron energies and a minimum at low energies below the positronium formation threshold. This minimum is very sharp for Ne and becomes progressively shallow for the heavier noble gas atoms. At very small energies the cross section rises very strongly indicating the existence of a virtual level for the positron. We note also the rapid rise of the cross sections as positronium formation channels open.

There is significant scatter in the experimental data for grand total cross sections. Similarly, previous theoretical calculations (all of them are single-channel methods) show large variations depending on the accuracy with which the polarization potential is modeled. We refer to [3, 4, 5] for detailed discussion and note here only that generally the CCC calculations are in good agreement with the measurements. For example, the CCC calculations for Ne in particularly good agreement with the measurements of Charlton et al. [14] and Stein et al. [17] in the energy region just below postronium formation. The region between positronium formation and
Figure 2. Differential cross section for positron scattering from Xe. Theoretical results are present CCC, Sin Fai Lam [13] and ROP results are due to McEachran [5] (ROP). The experimental results are due to Machacek et al. [5].

Figure 3. Grand total cross section for positron scattering from Ne. The experimental data are due to Jones et al. [3], Charlton et al. [14], Sinapius et al. [15], Coleman et al. [16], Stein et al. [17], Jaduszliwer and Paul [18], Canter et al. [19]. The present theory is labeled CCC, and the other is due to Baluja [20].
ionization thresholds, where the single-centre CCC method cannot describe the scattering, has been excluded from the calculations.

4. Conclusions
We have developed a single-centre CCC method for positron scattering from noble gases. The target states have been generated in the frozen core approximation, where only one-electron excitations from the $p^6$ shell are allowed. We analyzed the accuracy of the model, and presented a simple way to improve it using a model polarization potential. Large close-coupling calculations have been conducted to obtain convergent results for positron scattering from noble gases. Results for elastic differential cross sections and grand total cross section have been presented and found to be generally in good agreement with experiment.

The present (single-centre) formulation of the CCC method does not allow for (accurate) calculation of scattering process in the region between positronium formation and ionization thresholds. At energies above the ionization threshold, the positronium channels are incorporated indirectly via positive-energy atomic states of large orbital angular momentum. In order to adequately describe positron-atom scattering at all energies a two-center formulation has to be adopted. Such formulation has been completed in our group for positron scattering from helium and quasi two-electron targets [10]. Extension to noble gas targets is planned in near future.

Acknowledgments
The work was supported by the Australian Research Council and the ARC Centre for Antimatter-Matter Studies. We are grateful for access to the Australian Computing
Figure 5. Grand total cross section for positron scattering from Kr. The experimental data are due to Makochekanwa et al. [4], Zecca et al. [24], Jay and Coleman [25], Sinapius et al. [15], Dababneh et al. [26]. Theoretical results as in Figure 3 and in addition due to Parcell et al. [27].

Infrastructure Facility and its Western Australian node iVEC.

References
[1] Surko C M, Gribakin G F and Buckman S J 2005 J. Phys. B 38 R57
[2] McAlinden M T and Walters H R J 1992 Hyperfine Interact. 73 65
[3] Jones A C L, Makochekanwa C, Caradonna P, Slaughter D S, Machacek J R, McEachran R P, Sullivan J P, Buckman S J, Stauffer A D, Bray I and Fursa D V 2011 Phys. Rev. A 83 032701
[4] Makochekanwa C, Machacek J R, Jones A C L, Caradonna P, Slaughter D S, McEachran R P, Sullivan J P, Buckman S J, Bellm S, Lohmann B, Fursa D V, Bray I, Mueller D, Stauffer A D and Hoshino M 2011 Phys. Rev. A 83 032721
[5] Machacek J R, Makochekanwa C, Jones A C L, Caradonna P, Slaughter D S, McEachran R P, Sullivan J P, Buckman S J, Bellm S, Lohmann B, Fursa D V, Bray I, Mueller D W and Stauffer A D 2011 New J. Phys. 13 125004
[6] Fursa D V and Bray I 1995 Phys. Rev. A 52 1279–1298
[7] Raichenko Y, Kramida A E, Reader J and NIST ASD Team 2011 NIST atomic spectra database (version 4.10)
[8] Radtsig A A and Smirnov B M 1985 Reference data on atoms, molecules and ions (Springer-Verlag)
[9] Fursa D V and Bray I 2012 New Journal of Physics 14 035002 URL http://stacks.iop.org/1367-2630/14/i=3/a=035002
[10] Umaturatov R, Kadyrov A S, Fursa D V, Bray I and Stelbovics A T 2010 J. Phys. B 43 125203
[11] Caradonna P, Jones A, Makochekanwa C, Slaughter D S, Sullivan J P, Buckman S J, Bray I and Fursa D V 2009 Phys. Rev. A 80 032710
[12] Fursa D V and Bray I 1997 J. Phys. B 30 5895–5913
[13] Sin Fai Lam I, T 1982 J. Phys. B 15 143–153
[14] Charlton M, Laricchia G, Griffith T C, Wright G L and Heyland G R 1984 J. Phys. B 17 4945
[15] Sinapius G, Raith W and Wilson W G 1980 J. Phys. B 13 4079
[16] Coleman P G, McNeill J D, Diana L M and Burciaga J R 1979 Phys. Rev. A 20(1) 145–153
Figure 6. Grand total cross section for positron scattering from Xe. The experimental data are due to Machacek et al. [5], Sinapius et al. [15], Dababneh et al. [26]. Theoretical results as in Figure 3 and in addition due to Parcell et al. [27].

[17] Stein T S, Kauppila W E, Pol V, Smart J H and Jesion G 1978 Phys. Rev. A 17(5) 1600–1608
[18] Jaduszliwer B and Paul D A L 1974 Appl. Phys. 3 281–284
[19] Canter K F, Coleman P G, Griffith T C and Heyland G R 1973 J. Phys. B 6 L201
[20] Baluja K L and Jain A 1992 Phys. Rev. A 46 1279–1290
[21] Zecca A, Chiari L, Trainotti E, Fursa D, Bray I and Brunger M 2012 J. Phys. B 45 015203
[22] Karwasz G P, Pliszka D and Brusa R S 2006 Nucl. Instr. and Meth. B 68 68
[23] Kauppila W E, Stein T S and Jesion G 1976 Phys. Rev. Lett. 36(11) 580–584
[24] Zecca A, Chiari L, Trainotti E, Fursa D, Bray I and Brunger M 2011 Eur. Phys. J. D 64(2) 317–321
[25] Jay P M and Coleman P G 2010 Phys. Rev. A 82(1) 012701
[26] Dababneh M S, Kauppila W E, Downing J P, Laperriere F, Pol V, Smart J H and Stein T S 1980 Phys. Rev. A 22(5) 1872–1877
[27] Parcell L A, McEachran R P and Stauffer A D 2002 Nucl. Instr. and Meth. B 192 180–184