J. Phys. B: At. Mol. Opt. Phys. **33** (2000) 2955–2963. Printed in the UK PII: S0953-4075(00)50885-2

Direct ionization of low-charge Li-like ions using a small pseudo-state basis

N R Badnell† and D C Griffin‡

† Department of Physics and Applied Physics, University of Strathclyde, Glasgow G4 0NG, UK
‡ Department of Physics, Rollins College, Winter Park, FL 32789, USA

Received 26 May 2000

Abstract. We have calculated cross sections for the direct ionization of Be^{+}, B^{2+} and C^{3+} by electron impact using a small pseudo-state basis within the R-matrix method (RMPS). On using one pseudo-state per l to represent the continuum, close agreement with converged RMPS results is obtained at energies $\gtrsim 3$ times the ionization limit provided that the cross sections to the pseudo-continuum are projected back onto the physical continuum. On using two pseudo-states per l, the close agreement is extended back down to energies below the ionization peak, again, provided that projection is used. The use of a small pseudo-state basis is necessary to describe ionization processes in more complex systems.

1. Introduction

In the last few years, several *ab initio* theoretical methods have been developed which, for the first time, have the capability of producing accurate electron-impact ionization cross sections. Common to all of the methods is the coupling of the initial states (before ionization) to the final states (after ionization). The convergent close-coupling (Bray and Stelbovics 1993), the hyperspherical close-coupling (Kato and Watanabe 1995), the R-matrix with pseudo-states (Bartschat and Bray 1996), the time-dependent close-coupling (Pindzola and Robicheaux 1996) and the exterior complex scaling (Rescigno *et al* 1999) methods have all produced ionization cross sections for hydrogen in excellent agreement with experiment. The convergent close-coupling (Bray and Fursa 1996), R-matrix with pseudo-states (Hudson *et al* 1996) and time-dependent close-coupling (Pindzola and Robicheaux 2000) methods have also produced accurate cross sections for the electron-impact ionization of helium, while the time-dependent close-coupling and R-matrix with pseudo-states methods have also been applied successfully to Li^{+} (Pindzola *et al* 2000). The direct (outer-shell) ionization of low-charge Li-like ions (Bray 1995, Bartschat and Bray 1997, Pindzola *et al* 1997, Marchalant *et al* 1997, Woitke *et al* 1998, Mitnik *et al* 1999, Scott *et al* 2000) and Na-like ions (Badnell *et al* 1998) has also been studied extensively and good agreement with experiment has been obtained, in general. These calculations are computationally demanding and the same methodology cannot be applied directly to more complex systems or ionization processes, such as excitation–autoionization. In the latter case, for example, the treatment of direct ionization is drastically simplified so as to focus on indirect processes (Berrington *et al* 1997, Berrington and Nakazaki 1998, Teng *et al* 2000). Since accurate electron-impact ionization cross sections for atomic ions are needed for the modelling of a variety of laboratory and astrophysical plasmas, it is important to extend the range of atomic systems that can be treated by these advanced methods. In this paper, we

0953-4075/00/162955+09$30.00

investigate the accuracy of using small pseudo-state bases to describe direct ionization. We compare our cross sections with converged RMPS results for the Li-like ions Be^+, B^{2+} and C^{3+} which were previously computed by ourselves and co-workers. Here we use the same type of pseudo-states (Laguerre) but just reduce their number. However, we now ensure that all pseudo-states lie above the ionization limit and, preferably, below the energy range of interest, as it is difficult to describe direct ionization by a small set of resonances. Also, we must project the excitation cross sections to the pseudo-continuum back onto the physical continuum since the pseudo-continuum can be expected to partially represent physical discrete states as well in this instance.

The structure of this paper is as follows: the RMPS method that we apply to ionization is reviewed in section 2 and the results of the present study are compared with those of converged RMPS calculations in section 3. We finish with a short conclusion.

2. Theory

We use an L^2-basis to represent the bound and continuum states of the ion (see, e.g., Yamani and Reinhardt 1975). Excitation of the positive-energy states corresponds to ionization. A more accurate approach, especially on using small bases, is to project the positive and negative energy L^2 states onto the true physical continuum.

We use the program AUTOSTRUCTURE (Badnell 1986) to generate an orthogonal set of Laguerre basis orbitals by Schmidt orthogonalizing the following non-orthogonal basis:

$$P_{nl}(r) = N_{nl}(\lambda_{nl} Zr)^{l+1} \mathrm{e}^{-\lambda_{nl} Zr/2} L_{n+l}^{2l+1}(\lambda_{nl} Zr). \tag{1}$$

Here L_{n+l}^{2l+1} denotes an associated Laguerre polynomial, N_{nl} is a normalization constant and $Z = z + 1$, where z is the residual charge on the ion. The scaling parameters, λ_{nl}, can be used to vary the energy distribution of the pseudo-states. We use three different bases to enable us to study the accuracy of using small L^2-bases. For all three bases, we use physical orbitals for 1s through 3d. We then supplement these by one or two pseudo-states per l, with two different sets of scaling parameters in the latter case. We solve the close-coupling equations using the R-matrix method (Burke and Berrington 1993, Berrington *et al* 1995) as applied for use with pseudo-states following Gorczyca and Badnell (1997). We carried out LS-coupling calculations with exchange for $L = 0$–15 together with a small 'top-up' for higher L.

Following Gallaher (1974), we determine our ionization cross sections from

$$\sigma_{\mathrm{ion}} = \sum_{\overline{n}} \left[1 - \sum_{n} |\langle n|\overline{n}\rangle|^2 \right] \sigma_{\overline{n}}, \tag{2}$$

where $|\overline{n}\rangle$ denotes a positive or negative energy pseudo-eigenstate, $\sigma_{\overline{n}}$ is the excitation cross section (from the initial ground state) to $|\overline{n}\rangle$ and $\langle n|$ denotes a physical discrete eigenstate. The $|\overline{n}\rangle$ and $\langle n|$ are themselves configuration-mixed states of the original target basis resulting from diagonalization of the N-electron Hamiltonian. The sum over n is over all physical discrete states, which converges by $n \approx 30$. See Badnell *et al* (1998) for further details.

3. Results

Detailed comparisons have already been made between converged RMPS results and those of other methods, as well as with experiment, for Be^+ (Pindzola *et al* 1997), B^{2+} (Woitke *et al* 1998) and C^{3+} (Mitnik *et al* 1999, Teng *et al* 2000) and we will not repeat them here. Instead, we focus on the role of projection and the accuracy that can be obtained from a small pseudo-state basis, based on a comparison with converged RMPS results.

Table 1. Pseudo-state scaling parameters[a] and energies for Be^+, relative to the ground state. The ionization limit is at 18.211 eV.

	Basis 1		Basis 2		Basis 3	
$\overline{nl}$	λ_{nl}	Energy (eV)	λ_{nl}	Energy (eV)	λ_{nl}	Energy (eV)
$\overline{4s}$	1.063	31.7	1.008	22.6	1.1	19.0
$\overline{4p}$	0.957	28.6	0.923	21.4	1.1	21.7
$\overline{4d}$	0.942	22.4	0.906	18.6	1.1	19.2
$\overline{4f}$	1.680	33.7	1.424	21.5	1.5	19.9
$\overline{5s}$	—	—	1.288	108.9	1.1	48.3
$\overline{5p}$	—	—	1.164	73.1	1.1	45.9
$\overline{5d}$	—	—	1.137	48.9	1.1	38.9
$\overline{5f}$	—	—	1.654	62.1	1.5	50.3
$\overline{5g}$	1.500	32.4	1.500	32.4	1.5	32.4

[a] Scaling parameters for pseudo-orbitals are actually entered into AUTOSTRUCTURE as negative numbers.

Table 2. Pseudo-state scaling parameters and energies for B^{2+}, relative to the ground state. The ionization limit is at 37.931 eV.

	Basis 1		Basis 3	
$\overline{nl}$	λ_{nl}	Energy (eV)	λ_{nl}	Energy (eV)
$\overline{4s}$	0.986	61.9	1.1	43.0
$\overline{4p}$	0.935	58.2	1.1	46.4
$\overline{4d}$	0.912	44.7	1.1	40.2
$\overline{4f}$	1.566	64.9	1.5	41.9
$\overline{5s}$	—	—	1.1	115.6
$\overline{5p}$	—	—	1.1	100.3
$\overline{5d}$	—	—	1.1	84.5
$\overline{5f}$	—	—	1.5	110.2
$\overline{5g}$	1.500	70.0	1.5	70.0

3.1. Be^+

In table 1, we give the scaling parameters and resulting pseudo-state energies for the three bases that we studied for Be^+. Basis 1 used one pseudo-state per l with the scaling parameters, λ_{nl}, optimized on KLL autoionizing states following Berrington *et al* (1997, table 2). Basis 2 used two pseudo-states per l (the $\overline{g}$ state excepted) optimized on the same autoionizing states. The optimization procedure does not ensure that the pseudo-states lie in the continuum (although they do so here). Basis 3 used two pseudo-states per l but this time the scaling parameters were simply set by hand so as to illustrate the relative insensitivity to them, provided that the pseudo-states remain above the ionization limit, i.e. optimization is not necessary.

In figure 1, we present results for excitation to the individual pseudo-states of Basis 1, both unprojected and projected. We see that excitation to the $\overline{4d}$ dominates and that it is subject to the largest reduction following projection. The projection factors—the sum over n in equation (2)—are 0.369, 0.213, 0.171, 0.055 and 0.136 for $\overline{4d}$, $\overline{4p}$, $\overline{4s}$, $\overline{5g}$ and $\overline{4f}$, respectively.

In figure 2(*a*), we compare our results from Basis 1 with the converged RMPS results of Pindzola *et al* (1997). We see that the unprojected results are an overestimate by $\gtrsim$30% at high energies but that the projected results agree closely with the converged (and linearly extrapolated) RMPS results from about $\sim$3 times the ionization limit and upwards. At lower

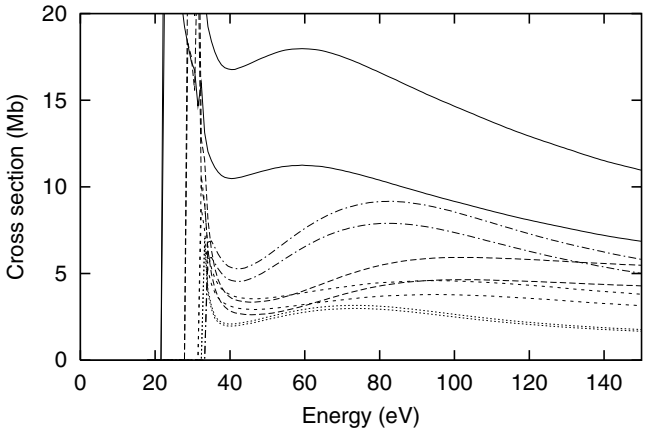
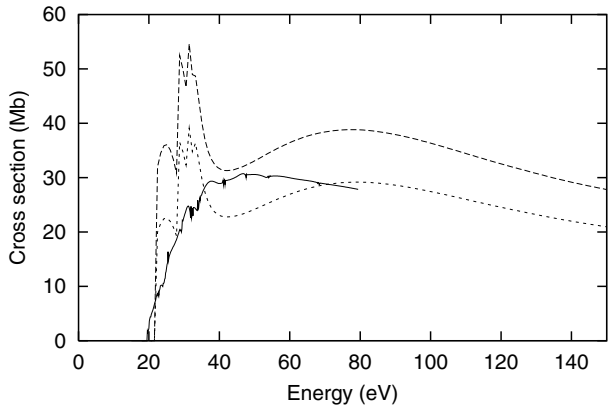


Figure 1. Electron-impact excitation cross sections to the basis 1 pseudo-states, $\overline{nl}$, of Be^+. For each pair of curves, the upper one represents the unprojected results and the lower one the projected results (all this work). ——, $\overline{4d}$; — · —, $\overline{4f}$; – – –, $\overline{4p}$; - - - -, $\overline{4s}$; · · · · · ·, $\overline{5g}$.

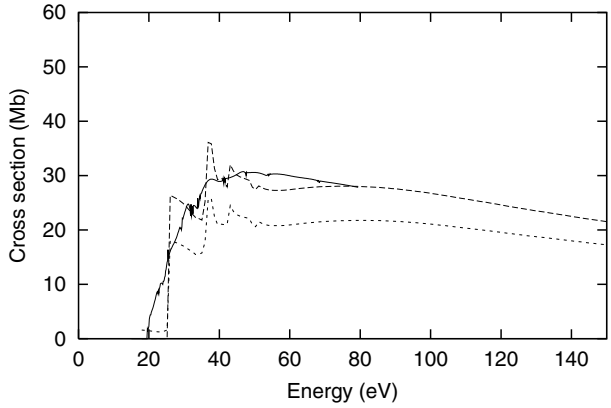
energies, they progressively worsen though. We note that the presence of the $\overline{5g}$ state produced a small (8%) but non-negligible increase in the total cross section compared to results calculated without it (not shown).

In figure 2(*b*), we show the results (for direct ionization only) of Berrington *et al* (1997) that we re-computed using their Slater-type orbital (STO) pseudo-states, which corresponds to our Basis 1 but without the $\overline{5g}$ state. Berrington *et al* also used a bound pseudo-$\overline{3p}$ state (which they labelled $\overline{2p}$) while we use a physical 3p state. This just means that our continuum $\overline{4p}$ state contains more bound character but, since we are going to project in any case, it is of little consequence to our approach. We note that our ground-state dipole polarizability (3p + $\overline{4p}$, only) differs by less than 10% from theirs. We see that our re-computed unprojected results of Berrington *et al* (1997) are in good agreement at high energies with the converged RMPS results but that our projection reduces them significantly (20%). This is due to the reduction of excitation to their $\overline{d}$ and $\overline{f}$ pseudo-states. If we compare our pseudo-state energies (table 1, Basis 1) with those of Berrington *et al* (1997, table 1), we see that our pseudo-state energies are significantly lower than theirs, the $\overline{p}$ pseudo-state excepted, even though we optimized our pseudo-state scaling parameters on the same KLL autoionizing states as them. Also, we find little sensitivity to just which autoionizing state is chosen to optimize on. If we manually adjust our scaling parameters so that our pseudo-state energies line up with theirs, we then find that the resulting direct ionization cross sections are in very good agreement with theirs. Berrington *et al* (1997) did not project their results but the resulting overestimate is partially cancelled out by the underestimate due to the omission of a $\overline{g}$ state. Their direct ionization cross sections are of reasonable magnitude for use in their study of indirect processes, which was the main focus of their work.

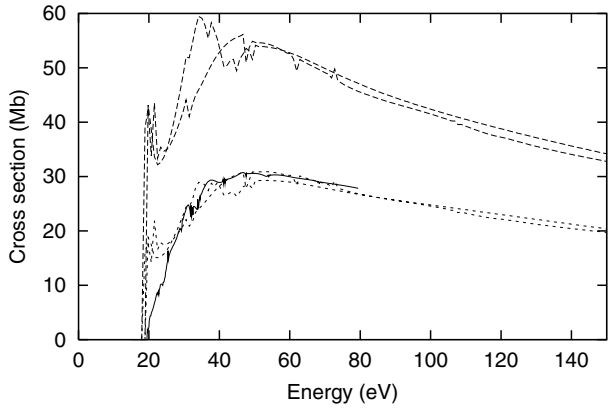
In figure 2(*c*), we present our results from Bases 2 and 3, both projected and unprojected. We see that projection has a large effect in both cases but that the results from Bases 2 and 3 differ little. Even more importantly, we see that the use of two pseudo-states per l extends the good agreement with the converged RMPS results to much lower energies than was obtained with a single pseudo-state per l in the continuum (Basis 1, figure 2(*a*)).



(*a*)

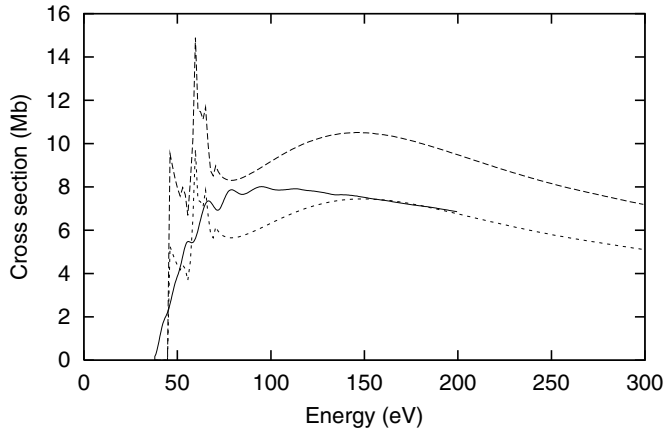


(*b*)

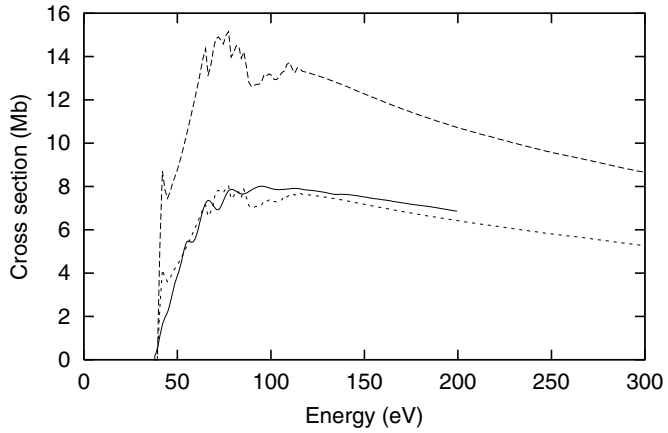


(*c*)

Figure 2. Direct electron-impact ionization cross sections for Be^+. ——, converged pseudo-state *R*-matrix results (Pindzola *et al* 1997); – – –, unprojected (this work); - - - -, projected (this work). (*a*) Basis 1; (*b*) re-computed using STOs of Berrington *et al* (1997); (*c*) Bases 2 and 3.



(*a*)



(*b*)

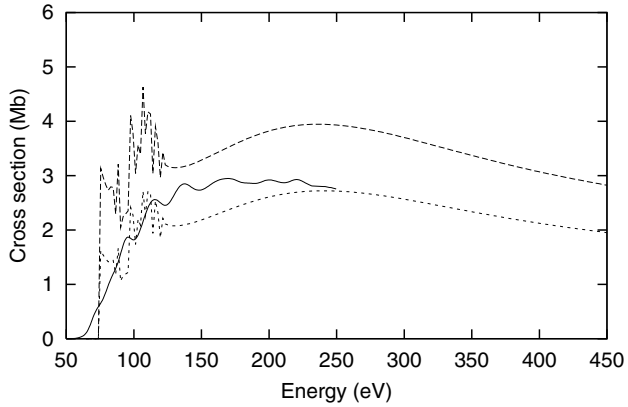
Figure 3. Direct electron-impact ionization cross sections for B^{2+}. ——, converged pseudo-state *R*-matrix results (Woitke *et al* 1998); – – –, unprojected (this work); - - - -, projected (this work). (*a*) Basis 1; (*b*) Basis 3.

3.2. B^{2+}

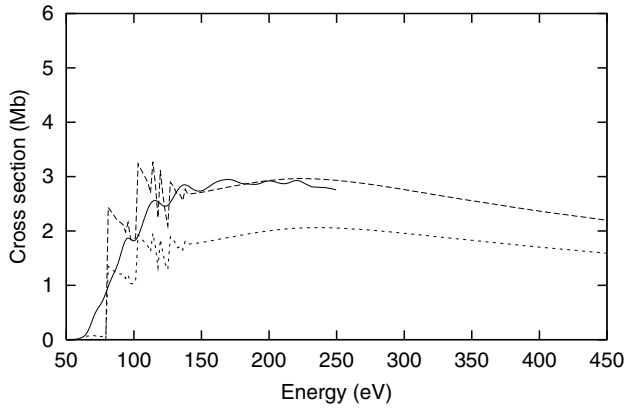
In table 2, we give the scaling parameters and resulting pseudo-state energies for B^{2+} for the two bases for which we present results. Given the results for Be^{+}, there is no need to use (the optimized) Basis 2 now.

In figure 3(*a*), we compare our results from Basis 1 with the converged RMPS results from Woitke *et al* (1998). We see that the unprojected results overestimate by $\gtrsim$40% at high energies but that the projected results agree closely with the converged RMPS results from about $\sim$3 times the ionization limit and upwards. Again, at lower energies they progressively worsen though.

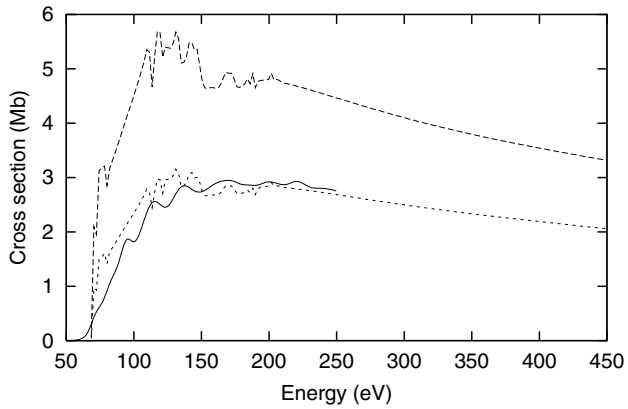
In figure 3(*b*), we present our results from Basis 3. The unprojected results are a factor of 2 too large but the projected results are again in close agreement with the converged RMPS results over a wide range of energies.



(*a*)



(*b*)



(*c*)

Figure 4. Direct electron-impact ionization cross sections for C^{3+}. ——, converged pseudo-state *R*-matrix results (Mitnik *et al* 1999); – – –, unprojected (this work); - - - -, projected (this work). (*a*) Basis 1; (*b*) re-computed using STOs of Teng *et al* (2000); (*c*) Basis 3.

Table 3. Pseudo-state scaling parameters and energies for C^{3+}, relative to the ground state. The ionization limit is at 64.494 eV.

	Basis 1		Basis 3	
$\overline{nl}$	λ_{nl}	Energy (eV)	λ_{nl}	Energy (eV)
$\overline{4s}$	0.944	102.6	1.1	77.5
$\overline{4p}$	0.919	96.9	1.1	80.4
$\overline{4d}$	0.899	74.6	1.1	68.6
$\overline{4f}$	1.541	109.7	1.5	71.5
$\overline{5s}$	—	—	1.1	208.7
$\overline{5p}$	—	—	1.1	175.9
$\overline{5d}$	—	—	1.1	147.9
$\overline{5f}$	—	—	1.5	192.9
$\overline{5g}$	1.500	121.5	1.5	121.5

3.3. C^{3+}

In table 3, we give the scaling parameters and resulting pseudo-state energies for C^{3+} for the two bases for which we present results.

In figure 4(*a*), we compare our results from Basis 1 with the converged RMPS results of Mitnik *et al* (1999). We see that the unprojected results overestimate by $\gtrsim$40% at high energies but that the projected results agree closely with the converged RMPS results from about $\sim$3 times the ionization limit and upwards. Again, at lower energies they progressively worsen though.

In figure 4(*b*), we show the results (for direct ionization only) of Teng *et al* (2000) that we re-computed using their STO pseudo-states. The methodology of Teng *et al* (2000) is the same as that used by Berrington *et al* (1997) and the pattern of results is also the same. Thus, we note the good agreement of our re-computed unprojected results of Teng *et al* (2000) with the converged RMPS results of Mitnik *et al* (1999) but also that our projection reduces them by 30%. Again, this would be partially cancelled out by the inclusion of a $\overline{g}$ pseudo-state.

In figure 4(*c*), we present our results from Basis 3. The unprojected results are again nearly a factor of 2 too large but the projected results are in good agreement with the converged RMPS results over a wide range of energies.

4. Conclusion

We have shown that small pseudo-state bases can accurately reproduce the direct ionization cross sections calculated with large converged pseudo-state bases for low-charge Li-like ions provided that the pseudo-states lie above the ionization limit and are projected back onto the physical continuum. Furthermore, our Basis 3 results suggest that the scaling parameters (i.e. pseudo-state distribution) determined for one ion can be used with little or no modification for (nearby) iso-electronic ions. The application of pseudo-states to describe ionization processes in more complex atoms, or indirect ionization processes even in simple systems, is only possible if small pseudo-state bases can be used.

Acknowledgments

In this work, NRB was supported by a UK PPARC grant (PPA/G/S/1997/00783) with the University of Strathclyde and DCG was supported by a US DoE Grant (DE-FG02-96-ER54367) with Rollins College.

References

Badnell N R 1986 *J. Phys. B: At. Mol. Phys.* **19** 3827–35
Badnell N R, Pindzola M S, Bray I and Griffin D C 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 911–24
Bartschat K and Bray I 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L577–83
——1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** L109–14
Berrington K A, Eissner W B and Norrington P H 1995 *Comput. Phys. Commun.* **92** 290–420
Berrington K A and Nakazaki S 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 313–27
Berrington K A, Pelan J and Quigley L 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 4973–90
Bray I 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** L247–54
Bray I and Fursa D V 1996 *Phys. Rev.* A **54** 2991–3004
Bray I and Stelbovics A T 1993 *Phys. Rev. Lett.* **70** 746–9
Burke P G and Berrington K A 1993 *Atomic and Molecular Processes—an R-matrix Approach* (Bristol: Institute of Physics)
Gallaher D F 1974 *J. Phys. B: At. Mol. Phys.* **7** 362–70
Gorczyca T W and Badnell N R 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 3897–911
Hudson E T, Bartschat K, Scott M P, Burke P G and Burke V M 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 5513–26
Kato D and Watanabe S 1995 *Phys. Rev. Lett.* **74** 2443–6
Marchalant P J, Bartschat K and Bray I 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** L435–40
Mitnik D M, Pindzola M S, Griffin D C and Badnell N R 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** L479–85
Pindzola M S, Mitnik D M, Colgan J and Griffin D C 2000 *Phys. Rev.* A **61** 052712(5)
Pindzola M S and Robicheaux F 1996 *Phys. Rev.* A **54** 2142–5
——2000 *Phys. Rev.* A **61** 052707(5)
Pindzola M S, Robicheaux F, Badnell N R and Gorczyca T W 1997 *Phys. Rev.* A **56** 1994–9
Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 *Science* **286** 2474–9
Scott M P, Teng H and Burke P G 2000 *J. Phys. B: At. Mol. Opt. Phys.* **33** L63–70
Teng H, Knopp H, Ricz S, Schippers S, Berrington K A and Müller A 2000 *Phys. Rev.* A **61** R060704(4)
Woitke O, Djurić N, Dunn G H, Bannister M E, Smith A C H, Wallbank B, Badnell N R and Pindzola M S 1998 *Phys. Rev.* A **58** 4512–12
Yamani H A and Reinhardt W P 1975 *Phys. Rev.* A **11** 1144–56