Iso-electronic trends for continuum coupling effects on the electron-impact excitation of H-like ions

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Abstract. We have carried out pseudo-state and non-pseudo-state R-matrix close-coupling calculations for the electron-impact excitation of the H-like ions He^+, Li^{2+}, Be^{3+} and B^{4+}. Illustrative results are presented for the ns $\rightarrow n'$s transitions since these are most affected by coupling to the continuum and highly excited states. In particular, our numerical results show that the effect of such coupling on the cross section scales roughly as $1/z$, where z is the residual charge on the ion.

1. Introduction

The spectroscopic modelling of non-LTE plasmas requires large amounts of accurate atomic data. International efforts such as the Opacity Project (Seaton 1987) and Iron Project (Hummer *et al* 1993) have sought to address those needs. The computations are based on solving the close-coupling equations using the standard R-matrix method (Burke and Robb 1975) as implemented in the RMATRX I code (Berrington *et al* 1995). While it is able to treat arbitrary atoms, allow for relativistic effects and include resonances in an efficient manner, the standard R-matrix method only uses a limited close-coupling expansion. The importance of coupling to highly excited states and the continuum has long been recognized (Castillejo *et al* 1960, Burke and Webb 1970) but not explored systematically until relatively recently even though Yamani and Reinhardt (1975) showed that the use of a finite L^2-basis (e.g. Laguerre) resulted in a Gaussian quadrature for the sum over bound and continuum states found in the close-coupling expansion. In 1992 Bray and Stelbovics demonstrated that convergence of the close-coupling expansion could be achieved for H on using a relatively small (~ 30) set of Laguerre pseudo-states. Subsequently, Bray and co-workers have studied a wide range of (mainly non-resonant) excitation and ionization phenomena in quasi one-electron neutral atoms with their convergent close-coupling method (CCC— Bray and Stelbovics 1992a, b), obtaining impressive agreement with experiment (see, for example, the review by Bray and Stelbovics (1995)).

Coupling to the continuum (and highly excited bound states) manifests itself at intermediate energies, which range roughly from the ionization limit to four or five times the ionization limit. Like the coupling effects observed on comparison of traditional close-coupling and distorted-wave results, the effect of coupling to the continuum is largest for neutral atoms and for the weakest transitions. But, given the large body of atomic data that is available and is being used that results from standard (non-pseudo-state) R-matrix calculations, it is important to study quantitatively a range of transitions, charge states and

collision energies so as to try to give guidance to users as to the validity of existing data. We focus on H-like ions as they are the least computationally demanding, enabling us to maximize our effort on the inclusion of pseudo-states. In any collisional–radiative model a complete set of transition data is required and it is not unusual for weaker (i.e. non-dipole) transitions to be the dominant populating mechanism for the upper state of an emission line. Thus, we focus on $ns \rightarrow n's$ transitions, and in particular $1s \rightarrow 2s$, $1s \rightarrow 5s$ and $4s \rightarrow 5s$ so as to contrast the effect of continuum coupling on both low- and high-lying states. From the work of Bubelev *et al* (1995), we do not expect continuum coupling effects to scale with n for these principal quantum numbers. If continuum coupling effects are sufficiently small for these $ns \rightarrow n's$ transitions in a given ion then it is likely to be true for dipole, quadrupole, etc transitions as well. The results should also be a pointer to the likely effect of continuum coupling in non-H-like ions, at least for spin-allowed transitions. Although we do not focus on resonances in particular in this work, we wish to pursue our studies using the *R*-matrix method since, currently, the associated computer codes are the most well developed for the generation of 'accurate' atomic data for collisional–radiative modelling.

Within the *R*-matrix approach, the intermediate energy *R*-matrix method (IERM) of Burke *et al* (1987) has sought to address continuum coupling by making a second *R*-matrix expansion, this time for the active atomic electron. Even in its reduced form (using a smaller expansion for the atom, see Scott and Burke (1993)) the IERM has yet to be applied beyond hydrogen. Adaptation of the standard *R*-matrix method to use a large pseudo-state expansion enables one to benefit from the large effort that has already gone into their general development. The practical difficulty lies in orthogonalizing the continuum basis to the pseudo-state basis. The original (recurrence relation) method for Schmidt orthogonalization is unstable when a large number of pseudo-states are used (Berrington *et al* 1995). This was overcome by Bartschat *et al* (1996b) who implemented an explicit numerical Schmidt orthogonalization procedure. We note that if we have NRANG1 (say) orthogonal pseudo-orbitals and NRANG2 orthogonal continuum basis orbitals then, in general, the combined orthogonal basis contains less than NRANG1 + NRANG2 orbitals. This manifests itself in the Schmidt orthogonalization by the occurrence of poles at large negative and/or positive energies, which must be discarded. Recently, Gorczyca and Badnell (1997) introduced an alternative approach, namely diagonalization of the matrix of overlaps between the two orthogonal bases. A zero eigenvalue corresponds to a transformation eigenvector that would generate a linearly dependent basis orbital and so this eigenvector is automatically discarded. We note that Gorczyca and Badnell (1997) have implemented this approach within the RMATRX I code while Bartschat *et al* (1996b) implemented their Schmidt orthogonalization procedure within the RMATRX II code (Burke *et al* 1994) which currently cannot describe photoionization or allow for relativistic effects, unlike RMATRX I. Of course, it is straightforward to implement the Schmidt orthogonalization procedure within RMATRX I, we have done so ourselves. Finally, we note that Berrington (1996, private communication) allows for a large pseudo-state expansion within the RMATRX I code by Lagrange orthogonalizing the continuum basis to all of the pseudo-orbitals. This necessitates the adjustment of the static potential that is used to generate the continuum basis, so as to compensate somewhat for the inclusion of an unphysical potential by the Lagrange multipliers.

The electron-impact excitation of low-charge H-like ions has been studied extensively. We note the studies that are most relevant to the present work. Abu-Salbi and Callaway (1981) carried out relatively small pseudo-state calculations for the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions in C^{5+} and O^{7+}. Over a wide range of energies for the $1s \rightarrow 2s$ transition they found large differences from the results of calculations that included little or no

coupling, but they did not establish the convergence of their pseudo-state expansion. For the 1s → 2p transition even the results of the Coulomb–Born approximation differed little from their pseudo-state results. Aggarwal and Kingston (1991) carried out 15-state *R*-matrix calculations for C^{5+} including only physical states up to $n = 5$ and obtained good agreement (< 5%) with the results of Abu-Salbi and Callaway (1981) for the 1s → 2s transition over the limited energy range of their calculation—up to 1.5 times the ionization limit. Aggarwal *et al* (1991) and Fon *et al* (1994) also carried out 15-state *R*-matrix calculations, this time for He^+. Bray *et al* (1993) carried out CCC calculations for He^+ which showed that the preceding (non-pseudo-state) *R*-matrix results substantially overestimated the cross section for the 1s → 2s transition over a wide range of energies above the ionization limit. However, Bray *et al* (1993) only carried out a limited resolution of the resonances. But, recently, Kisielius *et al* (1996) demonstrated the importance of resonances and their effect on low-temperature rate coefficients for He^+.

The organization of this paper is as follows. In section 2 we describe the pseudo-state basis that we use in our *R*-matrix calculations, its generation by the AUTOSTRUCTURE code (Badnell 1986), and the procedure that we use to orthogonalize the continuum orbitals to the pseudo-orbitals, as implemented by Gorczyca and Badnell (1997) within the RMATRX I code. In section 3 we compare our results from pseudo-state and non-pseudo-state *R*-matrix calculations for $ns \to n's$ transitions in He^+, Li^{2+}, Be^{3+} and B^{4+}. We finish with a short conclusion.

2. Theory

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

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

Here L_{n+l}^{2l+1} denotes an associated Laguerre polynomial (Abramowitz and Stegun 1972) and N_{nl} is a normalization constant. We note that the scaling parameter λ_{nl} does not include the nuclear charge Z (in general $Z = z + 1$, where z is the residual charge on the ion). We take all of the λ_{nl} to be equal to unity in all of our calculations since we find that this value minimizes the size of the pseudo-resonance structure, i.e. it speeds up the convergence of the pseudo-state expansion. We use physical orbitals for those states that we wish to study transitions between, rather than rely on using a large enough set of Laguerre states so as to converge to the physical ones. In a general atom N-electron configurations are built-up from the one-electron orbitals and then the Hamiltonian is diagonalized to obtain the set of N-electron eigenenergies and eigenstates. Thus, the full generality of AUTOSTRUCTURE can be used to determine the atomic structure as before.

We have two distinct sets of orthonormal orbitals, namely the atomic orbitals which we denote by $\bar{\mathbf{p}}$ and the continuum basis orbitals which we denote by $\mathbf{u}$—the latter set describes the scattering electron. We now form a single orthonormal set $\mathbf{v}$ which consists of $\bar{\mathbf{p}}$ plus a new continuum basis $\bar{\mathbf{u}}$ as follows: write $\bar{\mathbf{u}} = \mathbf{a}\bar{\mathbf{p}} + \mathbf{b}\mathbf{u}$, then $\mathbf{v}$ is orthonormal if $\mathbf{a} = -\mathbf{b}\mathbf{M}$ and $\mathbf{b} = \mathbf{O}/\sqrt{\mathbf{d}}$. Here, $\mathbf{M}$ is the matrix of overlap integrals between $\bar{\mathbf{p}}$ and $\mathbf{u}$, $\mathbf{O}$ is the matrix that diagonalizes $\mathbf{I} - \mathbf{M}^{\mathrm{T}}\mathbf{M}$, and $\mathbf{d}$ is the associated diagonal eigenvalue matrix. Eigenvalues of zero correspond to linear combinations of the $\mathbf{u}$ basis that are spanned by the $\bar{\mathbf{p}}$ basis and these are neglected (in practice, we keep those with eigenvalues greater than 10^{-4}, which we find is more than sufficient to avoid any numerical instability). Thus, in general, the new continuum basis $\bar{\mathbf{u}}$ contains less orbitals than the original $\mathbf{u}$ basis. However, care must be taken in evaluating the Buttle correction since the effective one-body Hamiltonian is not

diagonal in **v**, and so we diagonalize it. We then recover the original eigenenergies and surface amplitudes of the **u** basis plus some extra ones corresponding to that part of the **v** basis that is spanned by $\overline{\mathbf{p}}$, not by **u**. A more detailed exposition is given by Gorczyca and Badnell (1997). This procedure for obtaining a continuum basis that is orthogonal to the atomic basis is completely automatic and numerically stable with large numbers of pseudo-orbitals—up to 15 per angular momentum have been tested. In contrast, we find that the numerical Schmidt orthogonalization procedure begins to show numerical instabilities if too many pseudo-orbitals are included, especially with a large continuum basis. Bartschat *et al* (1996a) have noted similar problems.

With a numerically orthogonalized basis there is no simple representation of the second derivatives which are required for the evaluation of the matrix elements of the kinetic-plus-nuclear and mass–velocity plus Darwin operators. Bartschat *et al* (1996b) evaluated the second derivative numerically, for the kinetic-plus-nuclear operator present in RMATRX II. We take a different approach. We recognize that before any orthogonalization takes place each orbital ($R(r)$ say) of the **p** and **u** bases satisfies an equation of the form $R'' = Q(r)$. After orthogonalization each orbital then satisfies $\overline{R}'' = \overline{Q}$ where $Q \rightarrow \overline{Q}$ as $R \rightarrow \overline{R}$. The radial integrals of the kinetic-plus-nuclear and mass–velocity plus Darwin operators can easily be evaluated in terms of $\overline{Q}$.

3. Results

In all of our calculations we retained physical states up to $n = 5$. We carried out several calculations for He^+ so as to establish the pseudo-state expansion required to converge our cross sections to within a few per cent for the $n\text{s} \rightarrow n'\text{s}$ transitions over 3–13 Ryd. We first used 10 s-states and nine p-states, i.e. five pseudo-states per angular momentum in addition to our physical states. The addition of eight d-states did not significantly lower the cross sections any further neither did the addition of two extra s- and p- pseudo-states, except for the low-energy peak of the $1\text{s} \rightarrow 5\text{s}$ transition which we discuss in detail in section 3.2. Consequently, the calculations for the remaining ions used the 10 s-states and nine p-states target. Of the five pseudo-states per angular momentum, one is bound and four lie in the continuum. Adding two more per angular momentum still leaves only one bound, and six in the continuum. The non-pseudo-state calculations were carried out using only the physical states that were included in our pseudo-state calculations. We used 80 continuum basis orbitals per angular momentum which enabled us to go up to scattering energies of just over three times the ionization limit. We carried out exchange R-matrix calculations for total angular momentum $L = 0$–8 and non-exchange calculations for $L = 9$–60 for He^+ and $L = 9$–50 for the remaining ions. Transitions from the ground state ($1\text{s} \rightarrow n'\text{s}$) had largely converged by $L = 8$ but the higher L were important for transitions between highly excited states. Seaton's STGF code (see Berrington *et al* 1987) was used to solve the problem in the outer region and, given the strong coupling present, the results were spot checked against those obtained from the non-perturbative FARM code (Burke and Noble 1995). Finally, we note that the ionization limit is at Z^2 Ryd relative to the ground state of the ion, where Z is the nuclear charge of the ion.

3.1. 1s → 2s transitions

This transition in He^+ has been studied extensively because of the long-standing discrepancy between theory and experiment (see Seaton 1975). Bray *et al* (1993) showed that their CCC results removed the discrepancy except for energies a few eV above threshold. Bray *et al*

(1993) also found that their CCC results disagreed somewhat with their six-state close-coupling (6CC) results even below the lowest resonance (^1S_e at 44.8 eV), where energy resolution is not a problem, and attributed it to continued coupling to the continuum (and highly excited bound states) even at this low energy. Fon *et al* (1994) carried out 10- and 15-state (all physical states up to $n = 4$ and 5, respectively) close-coupling calculations and obtained the same qualitative cross section as from the 6CC below 44.8 eV (namely a shoulder in the cross section) and the same absolute cross section from both their 10CC and 15CC results. Fon *et al* found no evidence of the dip in the cross section that was found by Bray *et al* in their CCC results below 44.5 eV. We find that our pseudo-state *R*-matrix results are in very good agreement, both qualitatively and quantitatively, with the 15CC results of Fon *et al* (1994, figure 1) over 43–48 eV confirming that coupling to highly excited states and the continuum is indeed negligible here, between the $n = 2$ and $n = 3$ thresholds. We also obtain good agreement (a few per cent) with the CCC results of Bray *et al* (1993, figure 1) from above the ionization limit to three times the limit. Our pseudo-state *R*-matrix results for He$^+$, and for Li^{2+}, Be^{3+} and B^{4+}, are compared with our non-pseudo-state results in figure 1. We find that the dominant resonance structure is in agreement even for He$^+$ while above the ionization limit the collision strengths converge slowly with energy. Our pseudo-state results lie 17%, 10%, 7% and 5% below our non-pseudo-state results, respectively, for these four ions, at an incident energy equal to twice the ionization limit. However, if simpler approximations are used, such as distorted-wave or a small close-coupling expansion, then of course larger differences exist and persist to higher charge states. We illustrate this point
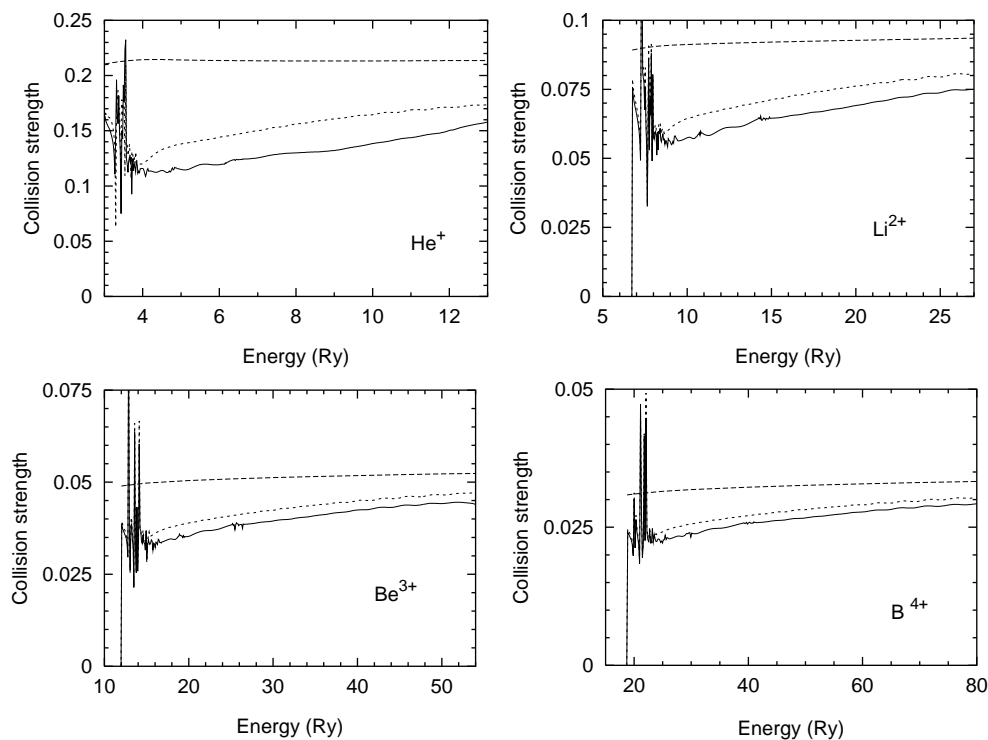

Figure 1. Electron-impact excitation collision strengths for the 1s → 2s transition in H-like ions. ——, pseudo-state *R*-matrix results; - - - -, non-pseudo-state *R*-matrix results; – – –, distorted-wave results. All this work.
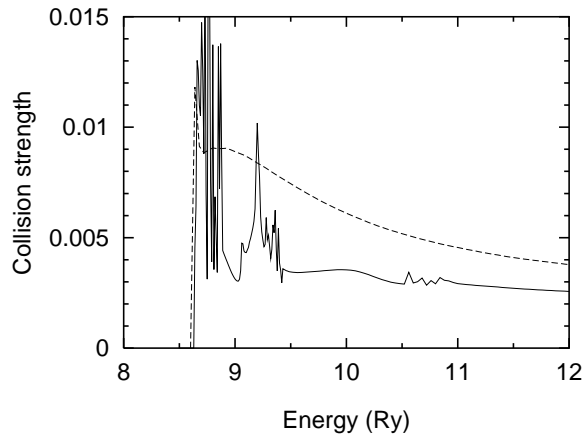
Figure 2. Electron-impact excitation collision strengths for the $1s \rightarrow 5s$ transition in Li^{2+}. ——, pseudo-state R-matrix results; – – –, non-pseudo-state R-matrix results. All this work.
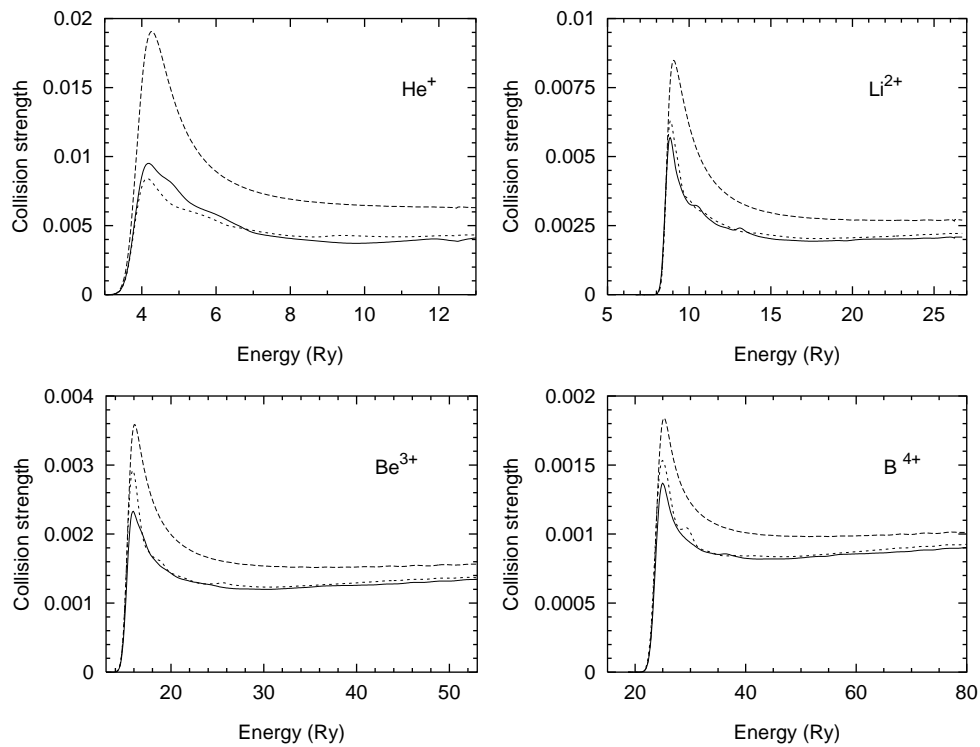

Figure 3. Electron-impact excitation collision strengths for the $1s \rightarrow 5s$ transition in H-like ions; convoluted with a 0.5 Ryd FWHM Gaussian function for He^+ and Li^{2+}, a 1 Ryd Gaussian for Be^{3+} and a 2 Ryd Gaussian for B^{4+}. ——, seven pseudo-states per angular momentum R-matrix results; - - - -, five pseudo-states per angular momentum R-matrix results; – – –, non-pseudo-state R-matrix results. All this work.

by the inclusion of (our) non-unitarized distorted-wave results in figure 1 as well—these still show a 20% difference from our pseudo-state results for the case of B^{4+}.

3.2. 1s → 5s transitions

The pseudo-state and non-pseudo-state results for this transition are quite different, qualitatively. In figure 2, for Li^{2+}, we see that the broad peak of the non-pseudo-state result dissolves into a set of pseudo-resonances. Similar behaviour is also found for the 1s → 4s transition (not shown) with the addition of a narrow Rydberg series of physical resonances converging on the $n = 5$ threshold. To obtain a meaningful comparison we have convoluted our collision strength for this transition with a narrow Gaussian function. If our pseudo-state expansion has converged then additional pseudo-states will change the magnitude, position and density of the pseudo-resonances but the convoluted result will remain unchanged. The collision strength just above threshold is also sensitive to the movement of pseudo-resonances that lie just above and/or below threshold, this can add or delete their contribution to this transition. In figure 3 we present our results that include seven pseudo-states per angular momentum as well as our results that include five pseudo-states per angular momentum. The addition of two extra (s- and p-) pseudo-states affects the collision strength only in a narrow energy range centred on the low-energy peak. In the case of He^+ this results in a small irregular increase over 4–6 Ryd while for Li^{2+}, Be^{3+} and B^{4+} we see that the peak is instead reduced a little over a very narrow energy range. The pseudo-state convergence is rather irregular here. Again we see that the differences between the pseudo-state and non-pseudo-state results persist over a wide range of energies. At twice the ionization limit our pseudo-state collision strengths lie 41%, 26%,
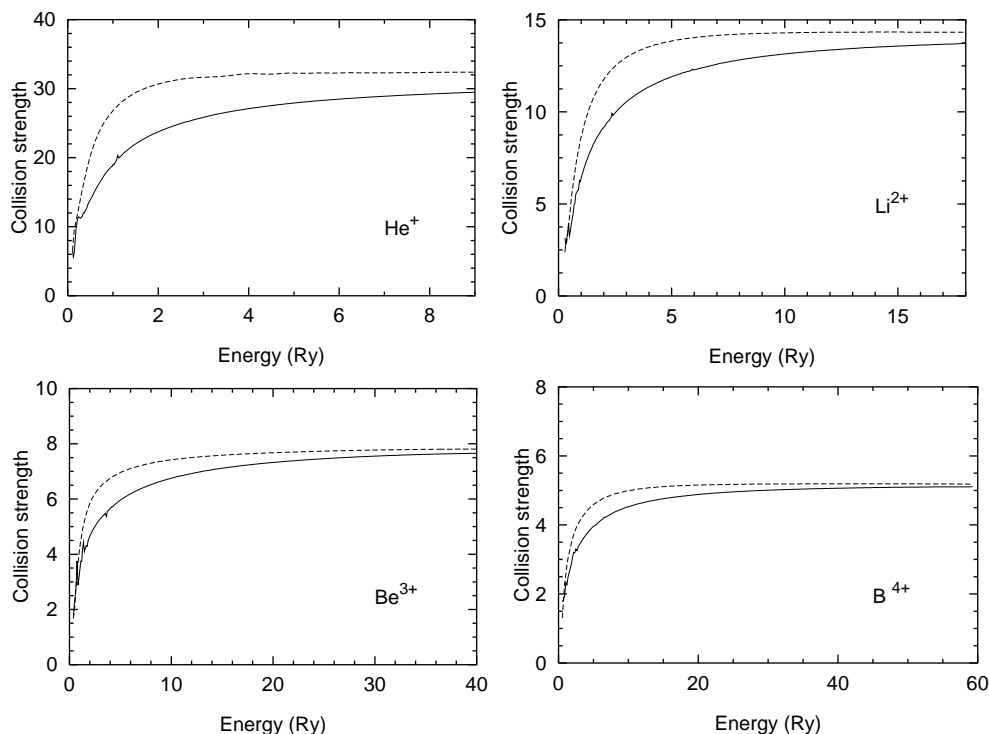

Figure 4. Electron-impact excitation collision strengths for the 4s → 5s transition in H-like ions. ——, pseudo-state R-matrix results; – – –, non-pseudo-state R-matrix results. All this work.

19% and 14% below our non-pseudo-state results, respectively, for the four ions considered here.

3.3. 4s → 5s transitions

Hydrogen atoms in the neutral beams that are used to heat a magnetic fusion plasma charge exchange with bare light-impurity ions and populate the $n = 4$ and $n = 5$ states. The subsequent photon emission provides an important diagnostic deep into the plasma—charge-exchange spectroscopy. Accurate cross sections between these highly excited states are of importance for determining the population of the excited states and hence the emissivity for a given diagnostic. In figure 4 we see that our pseudo-state and non-pseudo-state collision strengths converge more rapidly with energy than for transitions from the ground state; here the energy scale is relative to the initial 4s-state. At twice the ionization limit (now at $2Z^2 - 0.96Z^2$ Ryd) our pseudo-state collision strengths lie 16%, 9%, 6% and 4% below our non-pseudo-state results for He^+, Li^{2+}, Be^{3+} and B^{4+}, respectively. However, at lower energies the difference is much greater. Just below the plateau of the collision strength the difference is 30%, 20%, 16% and 12%, respectively, for these four ions. At the higher energies many more partial waves contribute to the collision strengths for this transition, recall that we needed up to $L \sim 50$ compared to $L \sim 10$ for the 1s → ns transitions.

4. Conclusions

We have compared the results of our pseudo-state and non-pseudo-state R-matrix close-coupling calculations for the electron-impact excitation of the H-like ions He^+, Li^{2+}, Be^{3+} and B^{4+}. The combination of a weak transition and a high-lying state means that the 1s → 5s transition shows the largest effect over a wide range of energies. In the case of the 4s → 5s transition, which involves two high-lying states, large effects are seen just above the ionization limit but being a stronger transition they rapidly decrease with energy. The effect of coupling to the continuum depends on how near the initial and/or final state is to the ionization limit, not just on the strength of the transition; this follows from contrasting our results for the 1s → 2s transition with those for the 1s → 5s transition. Surveying the percentage reductions in our non-pseudo-state results on the inclusion of pseudo-states to represent coupling to highly excited bound states and the continuum we note a roughly $1/z$ dependence, where z is the residual charge of the ion. Whilst these results give an indication of the validity of many existing (non-pseudo-state) R-matrix electron-impact excitation cross sections for positive ions, spin-forbidden transitions remain to be addressed as indeed do other processes such as photoionization.

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