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**LETTER TO THE EDITOR**

# Radiation damping in highly charged ions: an $R$-matrix approach

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**Abstract.** Using an $R$-matrix code recently developed by Robicheaux *et al* which includes a radiative optical potential, we have calculated electron-impact excitation cross sections to the $n = 2$ levels of $Fe^{25+}$ and $Mo^{41+}$. We focus on the $3lnl'$ resonance structure, which we find to be significantly damped even for low-lying resonances, and recent similar $R$-matrix calculations by Kisielius *et al* which omit radiation damping and significantly overestimate the resonance contribution. For dielectronic recombination resonances, we compare the extent of damping to a different $R$-matrix approach by Nahar and Pradhan, which uses the inverse of the photoionization process to calculate the radiative decay for low-lying resonances. It is demonstrated that the present method is superior for low-lying resonances, since the radiative width is incorporated in the total width for these resonances via the radiative optical potential.

Developments over the last few years of highly charged ion sources, such as SuperEBIT (see Knapp *et al* 1993) and heavy-ion storage rings, such as the one at GSI-Darmstadt (see Bosch 1987), have shed new light on the dynamics of highly charged ions. There are two effects which become ever more prominent as the nuclear or asymptotic ion charge ($Z$) increases, namely, relativistic effects and the effect of radiation damping on resonances. In principle, and in practice to a large extent, relativistic effects are treatable through the use of a Dirac representation (with or without the Breit interaction) and this has been implemented within a number of general codes to describe both atomic structure and collisions, for example, GRASP (Dyall *et al* 1989), MCDFB (Chen 1985) and DARC (Norrington and Grant 1987). Also, the less computationally demanding Breit–Pauli approximation has been implemented quite generally, for example the Iron Project $R$-matrix code (Berrington *et al* 1995) and AUTOSTRUCTURE (Badnell 1986). The situation with regard to the radiative damping of resonances is less satisfactory. It has long been known (Seaton 1969) that the non-resonant contribution to an electron-impact excitation cross section scales as $1/Z^4$ while, in the absence of radiation damping, the resonant cross section scales as $1/Z^3$. It has also long been recognized that resonances can be strongly radiation damped in highly charged ions, see e.g. Burgess (1964) and Davies and Seaton (1969).

Recently, using the standard $R$-matrix method, Kisielius *et al* (1995) studied the electron-impact excitation of the H-like ions $He^+$, $Fe^{25+}$ and $U^{91+}$ in the *absence* of radiation damping and noted strong low-lying resonances persisting even in $U^{91+}$. Also, recently, Zhang and Pradhan (1995) carried out a study of relativistic and radiation damping effects

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on *high-n* resonances present in the excitation of $Fe^{21+}$ and $Fe^{24+}$ ions. The purposes of this letter are to: (i) draw attention to the fact that even low-lying resonances are strongly affected by radiation damping in sufficiently highly charged ions; (ii) describe the general, automatic, *ab initio* approach to radiation damping of Robicheaux *et al* (1995) that we have implemented within the standard *R*-matrix approach—specifically within the asymptotic code STGF (see Berrington *et al* 1987)—and which applies to both low-lying *and* high-lying resonances; (iii) apply this approach to the resonant excitation and photorecombination (radiative plus dielectronic recombination) of $Fe^{25+}$ and $Mo^{41+}$ so as to demonstrate the importance of including radiation damping even for the lowest-lying resonances.

Radiation damping is easily and routinely included within (perturbation theory) calculations that make use of the independent processes and isolated resonance approximations. The independent processes approximation is quite good in general for multiply charged ions (see Badnell *et al* 1991, Pindzola *et al* 1992). However, while the isolated resonance approximation holds good in general for recombination (see Pindzola *et al* 1992) it can fail dramatically for excitation (see Badnell *et al* 1993). Even though the inclusion of higher-order terms within perturbation theory can alleviate this failure (see Badnell *et al* 1994) they are quite difficult to include generally in an *ab initio* manner. Furthermore, development of high energy resolution and state-selective recombination measurements further shows up failings in the second-order perturbative approach (see, for example, Pindzola *et al* 1995). Interacting resonances and interference between direct (non-resonant) and indirect (resonant) processes are automatically treated through the use of the close-coupling approximation for excitation and, through the weak-field approximation (see Henry and Lipsky 1967, Jacobs and Burke 1972), photorecombination/ionization. However, the radiative damping of resonances is not taken into account within this approach and its implementation via the *R*-matrix method. Studies of radiation damping using the *R*-matrix method have focused on resonances near the Rydberg limit. The (core) radiative width is independent of the principal quantum number ($n$) of the Rydberg electron while the autoionizing width and resonance separation both scale as $1/n^3$. Thus, for sufficiently high $n$, for any ion, the radiation field damps the resonances and smears them out. The Gailitis (1963) average, for excitation, was modified somewhat intuitively by Presnyakov and Urnov (1974) to allow for radiation damping. The radiation damping theory of Bell and Seaton (1985), carried out within the framework of quantum defect theory, put this on a more rigorous footing; their description did not quite correspond to that of Presnyakov and Urnov (1974) but no significant differences were noted in practice. Through the unitarity of the generalized *S*-matrix, the Bell and Seaton theory also gives rise to dielectronic recombination cross sections whose resonances are damped, smeared out and interacting. It should be noted that Bell and Seaton (1985) found no significant differences between the results of their theory and the original isolated resonance theory of Burgess (1964), when the resonances were averaged over a suitable energy range. The use of *R*-matrix theory scattering matrices within the Bell and Seaton (1985) theory is the basis of the damped *R*-matrix calculations of Pradhan and co-workers for high-*n* resonances in electron-impact excitation and dielectronic recombination (see, for example, Pradhan and Seaton 1985, Nahar and Pradhan 1994, Zhang and Pradhan 1995). Their treatment of low-*n* resonances is that of the standard *R*-matrix method, i.e. a neglection of the radiative width. We note that while dielectronic recombination via a $\Delta n = 0$ core excitation is dominated by high-*n* resonances, dielectronic recombination via a $\Delta n > 0$ core excitation and resonant excitation are both dominated by low-*n* resonances; essentially the cross section falls off as $1/n^3$ from the lowest energetically accessible $n$-state. It is the radiation damping of these low-lying resonances that needs to be addressed rather than the high-lying resonances.

In the present study, we have made use of the latest Iron Project (Hummer *et al* 1993) version of the Belfast *R*-matrix codes (Berrington *et al* 1995) which include spin–orbit, mass–velocity, and one-body Darwin relativistic corrections to the Hamiltonian (see Scott and Taylor 1982). In addition, we have modified the Hamiltonian further to include a non-local, imaginary, energy-dependent radiative optical potential to allow for the radiative decay of resonances. The derivation of this potential, as well as the strategy for handling the various types of decay, has been described by Robicheaux *et al* (1995). The use of this potential for electron-impact excitation calculations, as well as the specific modifications to the Belfast *R*-matrix codes, were detailed by Gorczyca *et al* (1995).

Briefly, the additional potential, in the length gauge, takes the form

$$V_{\rm rad} = -{\rm i}\sum_b \frac{2\omega_b^3}{3c^3} D|b\rangle\langle b|D \tag{1}$$

where $\omega_b = E - E_b$ is the energy difference between energies of the initial and final states, $D$ is the dipole operator and $|b\rangle$ represents a normalized final state. This potential contributes an additional term to the Hamiltonian matrix:

$$H_{\alpha\alpha'} \rightarrow H_{\alpha\alpha'} - {\rm i}\sum_b \frac{2\omega_b^3}{3c^3(2J+1)} \langle\alpha||r||b\rangle\langle b||r||\alpha'\rangle \tag{2}$$

where $J$ is the total angular momentum of the scattering-state symmetry. This accounts for decay to bound states $|b\rangle$ which are contained within the $R$-matrix box (all $1s^2$, $1s2l$ and $1s3l$ states in the present case). The use of this optical potential yields a non-unitary scattering matrix, $\mathbf{S}$, and the amount of damping is related to the non-unitary quantity $\mathbf{1} - \mathbf{S}^\dagger\mathbf{S}$ (Davies and Seaton 1969, Robicheaux *et al* 1995).

An alternative method for treating decay to inner-region states, as proposed by Nahar and Pradhan (1994), is to first calculate photoionization cross sections and then to compute the recombination cross section (which is proportional to the degree of damping, $\mathbf{1} - \mathbf{S}^\dagger\mathbf{S}$) using the detailed balance relationship

$$\sigma_{\rm RC} = \sigma_{\rm PI}\frac{g_{\rm i}}{g_{\rm f}}\frac{\omega^2}{c^2k^2}\,. \tag{3}$$

Here $\sigma_{\rm RC}$ and $\sigma_{\rm PI}$ are the partial recombination and photoionization cross sections, $g_{\rm i}$ and $g_{\rm f}$ are the statistical weights of the initial (bound) and final (continuum) levels, $\omega$ is the photon energy and $k$ is the electron momentum. As will be demonstrated, this procedure is only valid when the radiative width is much less than the autoionization width, since this method cannot incorporate the radiative width into the total width of the resonances when the final wavefunction is calculated in the absence of the radiative potential.

The second type of damping which must be considered in the present study is that of decay to higher-lying resonances, in particular the following processes: $1skl \rightarrow 3l'nl'' \rightarrow 1snl''$ ($n > 3$), where for pure $LS$-coupling, $l' = 1$, but in $JK$-coupling, other resonances may take part. As described by Robicheaux *et al* (1995) and Gorczyca *et al* (1995), this type of decay can be incorporated by modifying the the effective quantum number according to:

$$\nu_c = \frac{\nu}{\sqrt{1 - {\rm i}\Gamma\nu^2/Z^2}} \tag{4}$$

**Table 1.** Target energies (Ryd) for $Fe^{25+}$ and $Mo^{41+}$.

| level | $Fe^{25+}$ | $Mo^{41+}$ |
|---|---|---|
| $1s_{1/2}$ | 0.0 | 0.0 |
| $2s_{1/2}$ | 511.2 | 1352.1 |
| $2p_{1/2}$ | 511.2 | 1352.5 |
| $2p_{3/2}$ | 512.7 | 1361.8 |
| $3s_{1/2}$ | 606.3 | 1605.9 |
| $3p_{1/2}$ | 606.3 | 1606.0 |
| $3p_{3/2}$ | 606.8 | 1607.9 |
| $3d_{3/2}$ | 606.8 | 1608.2 |
| $3d_{5/2}$ | 606.9 | 1608.8 |

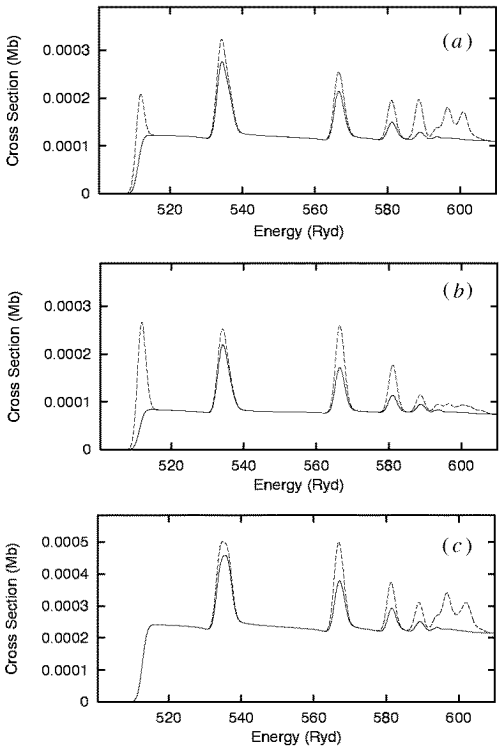


**Figure 1.** *R*-matrix calculation for the electron-impact excitation to the (*a*) $2s_{1/2}$, (*b*) $2p_{1/2}$, and (*c*) $2p_{3/2}$ levels in $Fe^{25+}$, convoluted with a 2.5 Ryd FWHM Gaussian; (- - - -), undamped; (——) damped.

where $\Gamma$ is the radiative width for the $3l'_j \rightarrow 1s_{1/2}$ core decay. By using a quantum-defect theoretical approach to compute a physical scattering matrix with this complex effective quantum number, this type of damping is completely incorporated:

$$\mathbf{S} = \mathcal{S}_{oo} - \mathcal{S}_{oc}\left(\mathcal{S}_{cc} - e^{-2\pi i\nu_c}\right)^{-1}\mathcal{S}_{co}\,. \tag{5}$$

This same basic strategy is used by Pradhan and Seaton (1985), although their formulation only agrees with ours provided that $\Gamma\nu^2/Z^2$ is small, then equation (4) becomes $\nu_c \sim \nu + i\Gamma\nu^3/2Z^2$.

The first system that we studied was the electron-impact excitation to the $n = 2$ levels of $Fe^{25+}$. The target energies used, which were obtained using the Breit–Pauli Hamiltonian (Scott and Burke 1980), are listed in table 1. Levels up to $n = 3$ were included in order

to provide the capture mechanism for the $3lnl'$ resonances. The resulting excitation cross sections with and without the radiative optical potential are shown in figure 1. For these calculations, we used 10 000 energy points over the energy range shown, and convoluted the cross sections with a 2.5 Ryd FWHM Gaussian in order to best portray the extent of damping. Note that the KL$n$ resonances, primarily the 2p$nl$ ($n \gtrsim 20$) ones just above the $2s_{1/2}$ and $2p_{1/2}$ thresholds, are completely damped, as are the KM$n$ resonances for $n \gtrsim 6$ ($E \gtrsim 590$ Ryd). More importantly, even the KMM resonances at $E \sim 535$ Ryd show roughly 10% damping.

We next repeated the above analysis for the case of electrons incident on $Mo^{41+}$. This system possesses an ionic charge which is high enough that significant damping is expected, yet low enough that our semi-relativistic treatment is still valid. We verified this by comparing our undamped excitation results to those obtained from a Dirac $R$-matrix calculation using the DARC suite of programs (Norrington and Grant 1987), and further verified that our treatment of damping was valid by comparing present dielectronic recombination results for the KLL resonances to those from a Dirac–Fock perturbative calculation (Zimmermann 1995); in both cases the agreement was excellent.

Excitation cross sections to the $n = 2$ levels are shown in figure 2, where we have now chosen a 10 Ryd FWHM Gaussian to convolute our 10 000 energy-points results. The effect of damping is expected to increase as the target ionic charge is increased, since the radiative rate scales as $\Gamma_r \sim Z^4 n^0$ for the type of damping presently considered, whereas the autoionization rate scales as $\Gamma_a \sim Z^0 n^{-3}$. This is found to be the case by comparing the $Mo^{41+}$ results in figure 2 with the $Fe^{25+}$ results in figure 1. In particular, the KMM resonances at about 1420 Ryd show more than a factor of 2 damping. As the charge state on the ion increases the damping factor increases further and by $U^{91+}$ we estimate, using AUTOSTRUCTURE, that the KMM resonances are damped by more than a factor of 20. Thus,

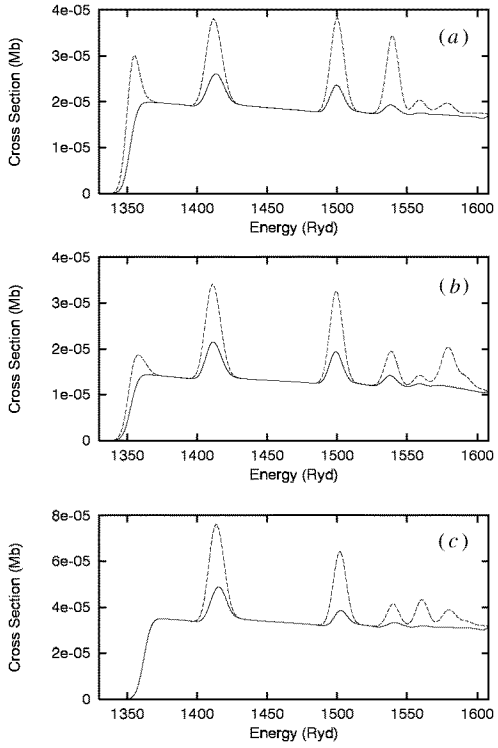


**Figure 2.** $R$-matrix calculation for the electron-impact excitation to the ($a$) $2s_{1/2}$, ($b$) $2p_{1/2}$ and ($c$) $2p_{3/2}$ levels in $Mo^{41+}$, convoluted with a 10 Ryd FWHM Gaussian; (- - - -) undamped; (——) damped.

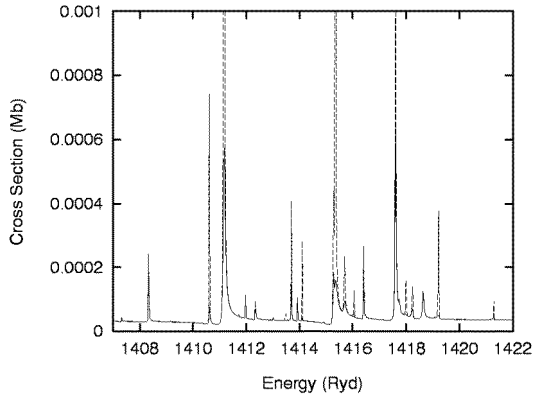


**Figure 3.** *R*-matrix calculation for the electron-impact excitation to the $2s_{1/2}$ level in $Mo^{41+}$ (unconvoluted); (- - - -) undamped; (——) damped.

the undamped resonance cross sections of Kisielius *et al* (1995) are likely to be a substantial overestimate. As demonstrated by Gorczyca *et al* (1995), these KMM resonances interact strongly with each other, and are therefore precisely the types of resonance which should be treated with non-perturbative methods, such as the present *R*-matrix method. Also, since the final 1s3*l* decay states are necessarily contained in the *R*-matrix box, the *R*-matrix itself must be modified as in equation (1).

In order to exemplify how the present method is perfectly suited for the treatment of this type of decay, and how the treatment of Nahar and Pradhan (1994) is not applicable for such a high-$Z$ ion, we focus on the 3s3p $^1P_1$ resonance in the 1s$k$p $\rightarrow$ 3s3p $\rightarrow$ 2s$k'$p excitation. The full, unconvoluted resonant cross section in the region of the 3$l$3$l'$ resonances is shown in figure 3, where the 3s3p $^1P_1$ resonance shows up as the large, broad feature at about 1411.5 Ryd. We do not show the complete extent of the undamped resonance for illustrative reasons, but it peaks at a maximum cross section of about 0.006 Mb, whereas the damped resonance peaks at about 0.0006 Mb, indicating a factor of 10 damping. More importantly, the width of this resonance is increased dramatically when damping is included. Perturbative calculations using AUTOSTRUCTURE determined that the radiative width is about an order of magnitude larger than the autoionizing widths to *each* continuum for this resonance, and there are four continua accessible to this resonance; these values are consistent with the degree of damping mentioned above. We next simplify the problem by focusing only on the $^1P_1$ partial wave, and include only the 3s3p configuration in the description of the KMM resonances, and only the 1s3s $^1S_0$ configuration for the final decay state. The dielectronic recombination cross section, which is proportional to the degree of damping, is shown in figure 4. Also shown is the result obtained by performing a photoionization calculation for the 1s3s $^1S_0 \rightarrow$ 3s3p $^1P_0 \rightarrow$ 2s$k'$p $^1P_1$ resonant process, and then using equation (3), as is done in the method of Nahar and Pradhan (1994). It is clearly seen that the dielectronic recombination cross section is about an order of magnitude too large, and therefore the degree of damping computed using that method is likewise an order of magnitude too large. From a perturbative perspective (see e.g. Robicheaux *et al* 1995), the inverse photoionization method amounts to using the following Lorentzian and energy-averaged expressions for the cross section

$$\sigma_{\mathrm{DR}} \sim \frac{\Gamma_{\mathrm{a}}\Gamma_{\mathrm{r}}}{(E - E_{\mathrm{res}})^2 + (\Gamma_{\mathrm{a}}/2)^2} \qquad \text{and} \qquad \langle\sigma_{\mathrm{DR}}\rangle \sim \frac{\Gamma_{\mathrm{a}}\Gamma_{\mathrm{r}}}{\Gamma_{\mathrm{a}}} \tag{6}$$

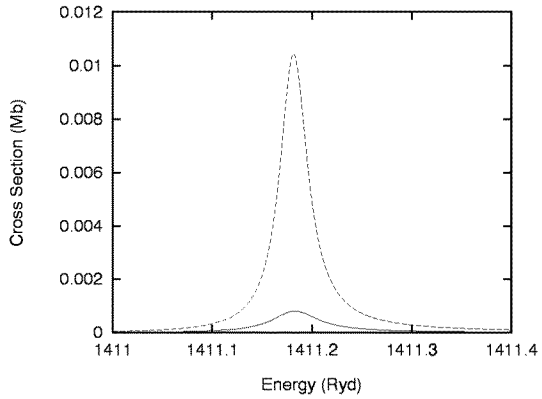


**Figure 4.** Dielectronic recombination cross section ($^1P_1$ partial wave only) in the vicinity of the $3s3p\,^1P_1$ resonance: (- - - -), results from a photoionization calculation; (——), results using the present radiative optical potential.

rather than using the *total* width in the denominator:

$$\sigma_{\rm DR} \sim \frac{\Gamma_{\rm a}\Gamma_{\rm r}}{(E-E_{\rm res})^2+(\Gamma_{\rm a}+\Gamma_{\rm r}/2)^2} \qquad \text{and} \qquad \langle\sigma_{\rm DR}\rangle \sim \frac{\Gamma_{\rm a}\Gamma_{\rm r}}{\Gamma_{\rm a}+\Gamma_{\rm r}}\,. \tag{7}$$

We note that neglect of the radiative width of a resonance is potentially more serious for dielectronic recombination than for resonant excitation, for which the cross section behaves like

$$\sigma_{\rm RE} \sim \frac{\Gamma_{\rm a}\Gamma_{\rm a}}{(E-E_{\rm res})^2+(\Gamma_{\rm a}+\Gamma_{\rm r}/2)^2} \qquad \text{and} \qquad \langle\sigma_{\rm RE}\rangle \sim \frac{\Gamma_{\rm a}\Gamma_{\rm a}}{\Gamma_{\rm a}+\Gamma_{\rm r}}\,. \tag{8}$$

Of course, if all of the radiative widths ($\Gamma_{\rm r}$) and all of the autoionizing widths ($\Gamma_{\rm a}$) satisfy $\Gamma_{\rm r} \gg \Gamma_{\rm a}$ then neglect of the radiative width causes the same overestimation factor in both dielectronic recombination and resonant excitation. However, a more realistic situation, particularly for low-lying $n$, is one where there is a combination of 'weak' resonances that satisfy $\Gamma_{\rm r} \gg \Gamma_{\rm aw}$ and 'strong' resonances that satisfy $\Gamma_{\rm r} < \Gamma_{\rm as}$. Consider the situation of two resonances each with the same radiative width $\Gamma_{\rm r}$ and with a single capture/autoionizing width of $\Gamma_{\rm aw}$ and $\Gamma_{\rm as}$, respectively. On using the energy-averaged form of equations (7) and (8), the dielectronic recombination cross section summed over both resonances is proportional to $\sim \Gamma_{\rm aw}+\Gamma_{\rm r} \sim \Gamma_{\rm r}$ and the resonant excitation cross section (the resonant part) is proportional to $\sim \Gamma_{\rm aw}\Gamma_{\rm aw}/\Gamma_{\rm r}+\Gamma_{\rm as} \sim \Gamma_{\rm as}$. Neglecting the radiative width (see equation (6)) results in a dielectronic recombination cross section proportional to $\sim \Gamma_{\rm r}+\Gamma_{\rm r}$ and a resonant excitation cross section proportional to $\sim \Gamma_{\rm aw}+\Gamma_{\rm as} \sim \Gamma_{\rm as}$. Although the contribution of the weak resonance to both dielectronic recombination and resonant excitation is overestimated by a factor $\Gamma_{\rm r}/\Gamma_{\rm aw}$, the weak resonance now contributes the same amount to the total dielectronic recombination cross section as the strong resonance, while having a negligible effect on the resonant excitation cross section. This potentially catastrophic overestimate of the dielectronic recombination cross section means that extreme caution must be exercised in obtaining dielectronic recombination cross sections (or for that matter, resonant photorecombination cross sections) from calculations that make use of the weak-field approximation for photoionization/recombination. The above analysis also

illustrates the reason why less attention has been paid to the radiation damping of resonances in excitation.

However, experimentalists are now able to produce bare uranium ($U^{92+}$) and so the first experiments on $U^{88+}$, $U^{90+}$, $U^{91+}$ etc (see, for example, Knapp *et al* 1995) are now coming online. At these high charge states even the lowest lying $n$ resonances are expected to be affected by radiation damping, based on perturbation theory, for both resonant excitation and dielectronic recombination.

In conclusion, we have demonstrated that the dominant low-lying resonances in electron-impact excitation and, even more so, in photorecombination/ionization can be strongly radiation damped and we have shown how damping of both low-lying *and* high-lying resonances can be incorporated in an automatic and *ab initio* manner within the $R$-matrix approach. The effects of radiation damping can now be included routinely within $R$-matrix calculations of collision cross sections for highly charged ions. The perturbative approach, using the independent processes and isolated resonance approximations, can be used to estimate their importance in the first instance for any particular reaction.

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