J. Phys. B: At. Mol. Opt. Phys. **31** (1998) L239–L248. Printed in the UK PII: S0953-4075(98)89020-2

LETTER TO THE EDITOR

Importance of radiation damping for low-lying photorecombination resonances

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Received 5 November 1997, in final form 13 January 1998

Abstract. We have implemented a multi-channel quantum defect theory approach within the asymptotic *R*-matrix codes (STGF and STGBF) which treats *all* closed channels as open. Furthermore, making use of this approach, we have implemented an *analytic preconvolution* of undamped *R*-matrix photoionization and photorecombination cross sections. This removes any doubt whatsoever as to whether the resonances are fully resolved or not. We show that fully resolved undamped *R*-matrix photorecombination cross sections are in very close agreement with undamped perturbative cross sections. We demonstrate, with explicit examples, the large and widespread effect of radiation damping on low-lying photorecombination resonances for H-like through Ni-like ions. This refutes the recent claims made by Pradhan and Zhang and validates the original work of Robicheaux *et al* and Gorczyca and Badnell with regard to the importance of radiation damping.

The effect of radiation damping of resonances in electron–ion collisions is currently a subject of great interest, and much dispute—see Robicheaux *et al* (1995), Gorczyca and Badnell (1996, 1997), Zhang and Pradhan (1995, 1997) and Pradhan and Zhang (1997) for a flavour of the debate. On the face of it, the issue would appear to be simple—perform calculations both with and without damping and note the effect. Alas, this is not the case. The first problem encountered is the actual inclusion of the effect of radiation damping—physically, this corresponds to the inclusion of the radiative width of a resonance, which causes the resonance profile to be broadened and the integrated cross section to be reduced. Whilst the inclusion of radiation damping is straightforward within the context of perturbation theory, it is not so within *R*-matrix theory. (The latter method is rightly regarded as our most accurate description of electron–ion collision processes, at least in the absence of radiation damping!) Thus, while one may compute and observe the effect of radiation damping perturbatively, its direct consequence for the results of *R*-matrix calculations is less clear; for example, are undamped perturbative results an accurate representation of undamped *R*-matrix results? A similar question can be asked with regard to damped results; however, the answer is even less clear here since there is disagreement over the actual form of the radiation-damped *S*-matrix. To try and make sense of the situation we first define our areas for discussion. Firstly, there is no disagreement for electron–electron transitions, i.e. resonant excitation. Except for the case of H-like and He-like ions, in general, one needs to go beyond the astrophysically important elements (those up to $\sim$ Fe) before radiation damping becomes significant. The key quantity for comparison here is that of the radiative width with the *strongest* autoionizing widths, and for the lowest-lying resonances since the resonant contribution to resonant excitation

0953-4075/98/050239+10$19.50

scales as $1/n^3$. The problem arises when we consider (resonances in) electron–photon transitions, i.e. photoionization and photorecombination. Methodologies and arguments that are valid for electron–electron transitions are not valid for electron–photon transitions: for example, extremely narrow resonances contribute significantly now and the competition (scaling) between autoionization and radiation behaves differently. We will return to these points later.

We now divide the electron–photon problem into two regions, a high-n one and a low-n one. We define the high-n region as that where the only important radiation damping is in the core (type-I damping); i.e. the Rydberg electron does not radiate and radiative recombination is negligible or, at best, can only be added in independently of the resonant (dielectronic) recombination. It is widely recognized that radiation damping is important here, for some non-trivial value of n, since the autoionizing width scales as $1/n^3$ (for fixed l), while the (core) radiative width is independent of n. The point at issue here has been the precise form of the high-n radiation-damped S-matrix. Robicheaux *et al* (1995) have demonstrated the formal equivalence between their optical potential theory and the radiation-damping theory of Davies and Seaton (1969). What has been puzzling is the difference between the final expression for the radiation-damped S-matrix of Robicheaux *et al* and that derived by Bell and Seaton (1985). As *emphasized* by Robicheaux *et al* in their original work, the practical difference between the two forms is utterly insignificant. There is no basis whatsoever for Pradhan and Zhang (1997) to claim that Robicheaux *et al* had reservations about the Bell and Seaton approach or for the implication that agreement between experiment and the results that they obtained using the Bell and Seaton formalism demonstrated the correctness of the Bell and Seaton S-matrix over the optical potential S-matrix. Indeed, Robicheaux (1998) has now identified (four) approximations made by Bell and Seaton in their derivation of the radiation-damped S-matrix. If these approximations are not made, then the S-matrix that results agrees *precisely* with that derived in an *ab initio* manner by Robicheaux *et al* (1995), and intuitively by Hickman (1984). We emphasize again that the approximate form of the high-n radiation-damped S-matrix derived by Bell and Seaton, and used extensively by Pradhan and co-workers, is a very accurate approximation.

Now we are left with the low-n problem (typically, $n < 10$) where, in general, the approach of Bell and Seaton (1985) or the type-I damping case of Robicheaux *et al* (1995) is insufficient. Here, both Rydberg and core damping may be important, along with radiative recombination, and the strongest autoionizing widths are typically orders of magnitude larger than the largest radiative widths. So why can radiation damping be important here for photoionization and photorecombination resonances when it is a negligible effect for resonant excitation? An answer has been given by Gorczyca and Badnell (1996). Briefly, it is not a comparison of the strongest autoionizing widths ($\Gamma_{\rm as}$) with the radiative width ($\Gamma_{\rm r}$) that is the key, it is the *weaker* autoionizing widths ($\Gamma_{\rm aw}$) which must be studied, specifically, those that satisfy $\Gamma_{\rm aw} \ll \Gamma_{\rm r}$. Assuming $\Gamma_{\rm r} < \Gamma_{\rm as}$, the resonant (dielectronic recombination) part of the photorecombination cross section for a weak resonance (including damping) is $\sim \Gamma_{\rm aw}$, while that for a strong resonance is $\sim \Gamma_{\rm r}$, and so the contribution from the weak resonance is negligible compared to that of the strong resonance. In the absence of radiation damping, the situation is transformed dramatically: the contribution of a weak resonance to the dielectronic recombination cross section is now $\sim \Gamma_{\rm r}$, *as big as* the contribution from even the strongest autoionizing resonance, which is still $\sim \Gamma_{\rm r}$. This model problem does not prove that radiation damping is important, but it demonstrates that arguments based on the strongest autoionizing widths alone are unsound; we note, in particular, the work of Pradhan and Zhang (1997) in this respect. Furthermore, the scenario described, that of the occurrence of 'weak' and 'strong' autoionizing widths, is very real. The change from LS to

intermediate coupling, for example, introduces weakly autoionizing resonances where there were none before. Such a situation arises even in LS coupling since the high-l autoionizing widths fall-off rapidly with l, where l is the angular momentum of the Rydberg electron.

We now see that it is important to carry out quantitative studies of radiation-damped and undamped photorecombination cross sections, at least to guide the way for R-matrix calculations—the effect of radiation damping is a non-problem from a perturbative point of view since it is always taken into account. Indeed, we have long been aware of the large effect of radiation damping on *perturbative* cross sections (some of which were reported by Gorczyca and Badnell (1996)). However, the size of the effect was such that we did not feel confident to assert that equally large effects should be omnipresent in R-matrix photorecombination cross sections. We have demonstrated the accuracy of the *damped* perturbative approach by comparison with experiment (see e.g. Badnell *et al* 1990), by analysis of the validity of the independent processes and isolated resonance approximations (Pindzola *et al* 1992) and, most recently, by comparison with radiation-damped R-matrix results (Gorczyca *et al* 1996). However, this does not prove that the undamped perturbative and R-matrix photorecombination cross sections would be, or should be, in equally good agreement, although we see no theoretical reason why this should not be so. However, the widespread use of undamped R-matrix photorecombination and photoionization cross sections (such as with the Opacity Project (Seaton 1987)) and the agreement with experiment for C^{4+} and Ar^{13+} (Pradhan and Zhang 1997, Zhang and Pradhan 1997) would seem to indicate otherwise. Recently (Gorczyca and Badnell 1997), however, we have revised our opinion—stimulated by the undamped R-matrix photorecombination results for Fe^{24+}, due to Zhang and Pradhan (1997), and their agreement and/or disagreement with damped perturbative results. Subsequently, we obtained excellent agreement between our damped perturbative and damped R-matrix results, and with experiment, for Fe^{24+} (see Gorczyca and Badnell 1997). We also noted large perturbative radiation-damping factors (two orders of magnitude) which were much larger than the factor of two or so difference between our damped R-matrix results and the undamped R-matrix results of Zhang and Pradhan (1997). On exploring the determination of undamped photorecombination resonances for Fe^{24+} we found that extremely narrow, but extremely high, resonances contributed significantly to the undamped R-matrix cross section, but contributed little to the damped cross section (precisely the situation described above in our weak versus strong resonance model). Millions of energies would be required to resolve each KLn group on using a constant step in energy or effective quantum number. Using only a few tens of thousands of such energies completely misses, let alone resolves, the myriad of narrow resonances that are present. Using perturbation theory to narrow down our search, we were able to determine a fully-resolved undamped R-matrix cross section for the KLL peak, but this rapidly became an impractical approach, even for the KLM peak. (An alternative approach is to search for the poles of the S-matrix in the complex plane, around the complex resonance energies; see Gorczyca *et al* (1996).) Nevertheless, these results indicated that undamped perturbative and undamped R-matrix photorecombination resonance cross sections could be brought into agreement, and that the damping factors were large—much larger than has been appreciated up until now perhaps, but that resolution of the undamped R-matrix resonances was the key issue. To be able to use perturbation theory as a reliable guide to R-matrix radiation-damping factors we need to be able to evaluate fully resolved undamped R-matrix photorecombination resonances efficiently, accurately, and reliably so as to be able to validate the undamped perturbative results. This we can now do, and we detail it next.

Our starting point is Seaton's unpublished R-matrix asymptotic codes STGB, STGF and STGBF (see Seaton (1981, 1985, 1986) and Berrington *et al* (1987) for some of the

background theory). We make use of multi-channel quantum defect theory. This method is a powerful tool for dealing with resonance structure but it has not been exploited as fully by the asymptotic codes used by the Belfast R-matrix suite of codes as by others, such as the JILA R-matrix suite (see e.g. Aymar *et al* 1996). In particular, its use has tended to be restricted to high-lying states such as found in connection with Bell and Seaton's (1985) damping theory or with Gailitis averaging. Indeed, Seaton (1983) has commented that the lack of widespread use in *ab initio* calculations is because it is not normally a good approximation to assume the non-Coulomb potentials to be of short range. However, its use with the R-matrix method means that it only need be applied outside of the R-matrix box. Furthermore, Gorczyca *et al* (1996) have shown how long-range open–open and open–closed multipole potentials can be incorporated within multi-channel quantum defect theory. In our approach we treat all closed channels as open. Deeply closed channels can give rise to some interesting numerical problems which we will not dwell on here; suffice to say that they are not intractable. The physical $\boldsymbol{S}$ and $\boldsymbol{D}$ matrices are written in terms of slowly-varying-with-energy unphysical $\boldsymbol{\mathcal{S}}$ and $\boldsymbol{\mathcal{D}}$ matrices as (Seaton 1983)

$$\boldsymbol{S} = \boldsymbol{\mathcal{S}}_{\mathrm{aa}} - \boldsymbol{\mathcal{S}}_{\mathrm{ab}} \left[\boldsymbol{\mathcal{S}}_{\mathrm{bb}} - \exp\left(-2\pi \mathrm{i}\nu\right) \right]^{-1} \boldsymbol{\mathcal{S}}_{\mathrm{ba}} \tag{1}$$

and

$$\boldsymbol{D} = \boldsymbol{\mathcal{D}}_{\mathrm{a}} - \boldsymbol{\mathcal{S}}_{\mathrm{ab}} \left[\boldsymbol{\mathcal{S}}_{\mathrm{bb}} - \exp\left(-2\pi \mathrm{i}\nu\right) \right]^{-1} \boldsymbol{\mathcal{D}}_{\mathrm{b}} \tag{2}$$

where ν denotes the effective quantum numbers and $\exp(\cdots)$ is a diagonal matrix. The partitioning (a, b) is usually taken to be open, closed (o, c) but we have implemented it in such a way that a contraction can take place followed by, for example, a Gailitis average. Electron-impact excitation cross sections are determined from $\boldsymbol{S}$ using the revised STGF code, while the unphysical $\boldsymbol{\mathcal{S}}$ matrices are passed to the revised STGBF code and the dipole $\boldsymbol{D}$ matrices computed, and hence a collision strength which can be converted to a photoionization or photorecombination cross section as desired. The unphysical $\boldsymbol{\mathcal{S}}$ and $\boldsymbol{\mathcal{D}}$ matrices are evaluated at several hundred energies and are then automatically interpolated at any desired collision energy so that the physical $\boldsymbol{S}$ and $\boldsymbol{D}$ matrices can be evaluated efficiently, using just equation (1) or (2), at as many energies as are required. However, even this becomes laborious when millions of energies are required as is the case, say, for the photorecombination of Fe^{24+}. Fortunately, we are now in a position to take advantage of an *analytic* preconvolution of the total photoionization cross section, originally developed for photoabsorption by Robicheaux (1993). This eliminates at root all problems associated with resolution. So long as we apply it below the first excited final state following photoionization, we can perform detailed balance and obtain photorecombination cross sections as usual. The total photoionization collision strength vector of initial states impacted-on by a photon, preconvoluted with a Lorentzian, is given by (Robicheaux 1993)

$$\boldsymbol{\Omega} = \frac{\mathrm{C}}{3} \left(\frac{\alpha\omega}{I_H} \right)^3 \mathrm{Re} \left[\boldsymbol{\mathcal{D}} \left(\frac{\boldsymbol{\mathcal{S}} + \mathrm{e}^{-2\pi \mathrm{i}\bar{\nu}^*}}{\boldsymbol{\mathcal{S}} - \mathrm{e}^{-2\pi \mathrm{i}\bar{\nu}^*}} \right) \boldsymbol{\mathcal{D}}^* \right] \tag{3}$$

where $\bar{\nu} = \nu / \sqrt{1 - \mathrm{i}\Gamma\nu^2/z^2}$ for closed channels and $\bar{\nu} = \mathrm{i}\infty$ for open channels, i.e. $\exp(-2\pi \mathrm{i}\bar{\nu}^*) = 0$. Here ω denotes the photon energy, I_H the ionization potential energy of hydrogen, α the fine-structure constant and $C = 1$ in intermediate coupling and $C = 2S + 1$ in LS coupling. The preconvolution works by introducing an arbitrary, constant, complex width (Γ) to broaden the resonances, just as in the case of radiation damping, but there is *no loss* associated with this procedure on using equation (3), only a redistribution. This is in contrast to the use of a complex energy to represent radiation-damping loss via, for

example, equation (1) with $\nu \rightarrow \bar{\nu}$. This powerful method completely eliminates the problem of resonance resolution and means that we can evaluate fully resolved undamped R-matrix photorecombination cross sections using only a few thousand physical energies. Currently, it cannot be applied to radiation-damped calculations—there is no way to redistribute the radiation damping as a loss term and keep a broadening-only non-loss term, at least using equation (3)—but radiation damping broadens the resonances naturally and so resolution is much less of a problem then. Currently, there is no partitioning by final state; only by summing over all final states is the full redistribution recovered. Note, there is no open–closed partitioning either. In fact, equations (1) and (2) do not factor-out the energy dependence of the $\boldsymbol{S}$ and $\boldsymbol{D}$ matrices for resonances that are fully contained within the R-matrix box (those formed by correlation configurations). We note that Lecomte *et al* (1994) have implemented a non-trivial scheme to do so in such a case. However, on using equation (3) we find that we only require $\sim$10 times as many 'unphysical' energies (i.e. several thousand) as before so as to obtain fully resolved preconvoluted results for this case as well. The preconvoluted undamped R-matrix calculations are now on the same footing as damped or undamped perturbative calculations that energy-average the Lorentz profile (if no energy averaging is carried out, then perturbative calculations suffer the same resolution problem of the resonance profiles).

Table 1. Photorecombination rate coefficients for Fe^{24+} at $T = 2$ keV (10^{-13} cm^3 s^{-1}).

	Undamped		Damped	
KLn	BPDW	BPRM	BPDW	BPRM
KLL	18.9	18.6	2.417	2.455
KLM	30.2	30.2	1.033	1.117
KLN	40.9	40.6	0.380	0.377
KLO	57.5	57.1	0.180	0.179
KLP	78.5	78.2	0.100	0.096

Our first results are Breit–Pauli photorecombination rate coefficients for Fe^{24+}, which we present in table 1; only the undamped R-matrix results are new but they are significant (see Gorczyca and Badnell (1997) for further details of the original work). We see that our undamped *preconvoluted* R-matrix results (BPRM) closely track our undamped perturbative results (BPDW), indeed, as closely as our damped R-matrix and perturbative results agree with each other. The undamped R-matrix results of Zhang and Pradhan (1997, table I) are a gross underestimate of the true fully resolved undamped cross section. The results in table 1 demonstrate that a comparison of undamped and damped perturbative results *can* accurately predict the effect of radiation damping on *fully resolved* undamped R-matrix photorecombination and photoionization cross sections. This is a powerful result since the perturbative calculations are extremely easy to perform. Indeed, only a single calculation of the relevant autoionization and radiative widths is required. This can be done using a general and fully automatic code such as AUTOSTRUCTURE (Badnell 1986), which we use here. The widths are then processed twice, once with the radiation-damping term, and once without. The size of the damping effect for Fe^{24+}—two orders of magnitude—means both that lower-charged He-like ions are significantly affected, as are other isoelectronic sequences. This we now demonstrate with explicit examples. In what follows, our statements about the effect of radiation damping refer to energy-integrated cross section peaks—the so-called resonance strength—rather than to the peaks of the cross sections

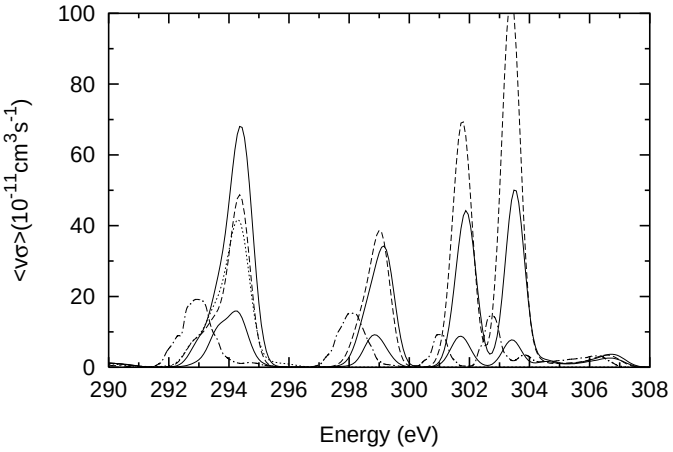

Figure 1. Photorecombination of C^{4+} for the KLn resonances, dominated by $n = 4$–7. Full curves, intermediate coupling perturbation theory, (upper) undamped and (lower) damped; broken curve, LS-coupling perturbation theory, undamped; dotted curve, LS-coupling preconvoluted R-matrix theory, undamped ($n = 4$ only)—all this work. Chain curve, undamped R-matrix theory of Pradhan and Zhang (1997). All cross sections have been convoluted with a 0.57 eV FWHM Gaussian function and multiplied by the electron velocity.

themselves, which can be misleading. The damping factor is the ratio of the undamped-to-damped integrated cross sections.

We present a series of results for C^{4+} in figure 1. We focus on the dominant KLN and higher resonances, initially. The four main peaks correspond to $n = 4$–7. Our radiation-damped results, R-matrix and perturbative—both LS and intermediate coupling, differ little from each other on the scale of the graph and so a single result is shown. We see that our undamped results show large factor differences from our damped results. For $n = 6$ and 7, the LS-coupling radiation-damping factor is significantly larger than the intermediate coupling factor, but the situation is reversed at lower n (in addition, the KLL and KLM damping factors are 1.84 and 1.86 in intermediate coupling, and 1.04 and 1.31 in LS coupling). This contrasting behaviour is a manifestation of the relative importance of spin–orbit mixing. As n increases, the fine-structure splitting of the core remains constant while the splitting of the $(N + 1)$-electron terms decreases. So, the spin–orbit interaction mixes LS-forbidden and LS-allowed autoionizing states more efficiently, relatively increasing the size of the LS-forbidden rates. It is interesting to note the slight drop in the undamped results just above the $2\,^3$S threshold (at about 298 eV) and the huge drop above the $2\,^1$S and $2\,^3$P thresholds (at about 304 eV). This can be understood in terms of the autoionization into excited states, the widths of which do not 'cancel', there being no corresponding dielectronic capture, and which then can dominate the radiative width. We see also that our undamped preconvoluted R-matrix results are in close agreement with our perturbative results, for the (LS-coupling) KLN peak. We cannot use equation (3) for higher energy peaks in this low-charge ion since that would take us above the first excited state ($2\,^3$S), but the KLN result suffices to validate the undamped perturbative results again. We show also in figure 1 the undamped R-matrix results of Pradhan and Zhang (1997). They used only 'several thousand photon energies' and so seriously underestimate the effect of radiation damping due to a substantial underestimate of the undamped cross section. Our radiation-damped R-matrix results are in good agreement with those of Pradhan and Zhang (1997) and with

experiment (Mannervik *et al* 1997, not shown) although, like their undamped results, the damped results of Pradhan and Zhang (1997) are ≈ 0.7 eV too low in energy compared to experiment. A full comparison between experiment and theory has been made by Pradhan and Zhang (1997), and by Schuch *et al* (1997) using our perturbative results, and so we do not pursue it further. We note that the radiation-damped method used by Pradhan and Zhang (1997) is not the same as the radiation-damped R-matrix method of Robicheaux *et al* (1995). Pradhan and Zhang (1997) follow the approach due to Sakimoto *et al* (1990). Undamped R-matrix photoionization calculations are performed to obtain dipole matrices which are then fitted to a known functional form (following Davies and Seaton 1969). These are then used to obtain a radiation-damped photoionization cross section. The main drawback to this approach, apart from having to fit all of the resonances involved, is that the functional form imposes (in effect) an additional approximation because it is not valid for resonances overlapping and interacting via their autoionizing width; it is valid for an overlap due to the radiative width alone. This 'isolated resonance' imposition is hardly in the spirit of the R-matrix method, in contrast to the optical potential radiation-damped R-matrix method of Robicheaux *et al* (1995). Nevertheless, in a simple system such as He-like ions this approach works well. This is not too surprising since our perturbation theory results agree closely with our R-matrix results as well.

Having seen the size of the effect of radiation damping on low-lying photorecombination resonances in He-like ions (and, by implication, H-like ions, e.g. the KLL peak for C^{5+} is damped by a factor of 1.57), we now turn to other sequences and present some illustrative results as a guide to the degree of damping that might be expected for Li-like through Ni-like ions. All of the perturbative results were computed in intermediate coupling, unless stated otherwise, and averaged over the fine-structure levels of the ground term. Where the damping factors are changing rapidly, with z or n, then small changes in the atomic structure may change the damping factors somewhat, but those presented here should be representative.

Li-like. The LMn damping factors for Fe^{23+} are 1.56, 1.69, 3.1 and 6.3 for $n = 3$–6. Lower-charge Li-like ions are also affected by damping; for example, for Mg^{9+}, the LMn damping factors are 1.07, 1.31 and 1.95 for $n = 4$–6. Also, a particular interest for Li-like ions concerns the relatively small energy separation of the 2s–2p$_J$ levels, which means that outer-electron stabilization is important for the lowest energetically accessible resonances formed by $\Delta n_c = 0$ core excitations. The damping factors (which cannot be obtained from type-I damping alone) for $n = 11$ and 15 are 1.10 and 1.30 for Ar^{15+} and are 1.33 and 1.36 for Fe^{23+}. Roughly 75% of the recombination is due to outer-electron stabilization for $n = 11$ and 50% for $n = 15$.

Be-like. For Fe^{22+}, while the damping factor for the LMn ($n = 3$) peak is only 1.18, the damping factors increase rapidly with n, namely 1.47, 2.7, and 4.7 for $n = 4$–6. For Mg^{8+}, the damping factors are 1.03, 1.32 and 1.60 for $n = 4$–6.

B-like. The addition of a 2p electron increases the damping significantly. For Fe^{21+}, the LMn peaks formed by $2p \rightarrow 3l$ promotions are damped by factors of 1.43, 2.4, 3.6 and 5.8 for $n = 3$–6. For Mg^{7+}, the damping factors are 1.06, 1.20, 1.44 and 2.0 for $n = 3$–6.

C-like. The 2p-promoted LMM peak for Fe^{20+} is damped by a factor of 1.24.

N-like. The 2p-promoted LMM peak for Fe^{19+} is damped by a factor of 1.32. Of particular interest, however, is photorecombination via the $2p^3\ {}^4S \rightarrow 2p^3\ {}^2P, {}^2D$ core excitations. This takes place purely via outer-electron stabilization. For Ne^{3+}, the damping factor for $n = 6$ is 1.49 and it varies quite slowly with n since both the autoionization and radiative widths scale as $1/n^3$. This example is illustrative of a more general class of problem—that of low-temperature photorecombination, which in many cases involves such a non-dipole core excitation. At high temperatures, the $2s \rightarrow 2p$ core excitation (in this case) dominates the total recombination of course.

O-like. The 2p-promoted LMM peak for Fe^{18+} is damped by a factor of 1.24.

F-like. The 2p-promoted LMn peaks for Fe^{17+} are damped by a factor of 1.31, 1.89, and 3.2 for $n = 3$–5. The damping factors for S^{7+} are 1.14 and 1.28 for $n = 3$ and 4, respectively, while for Mg^{3+} the LMM damping factor is 1.13. The ${}^2P_{3/2} \rightarrow {}^2P_{1/2}$ fine-structure transition in the core gives rise to a low-temperature photorecombination peak; again, the stabilization is purely via outer-electron transitions. For Fe^{17+}, this low-temperature peak opens up at $n = 18$ and is damped by a factor of 1.84.

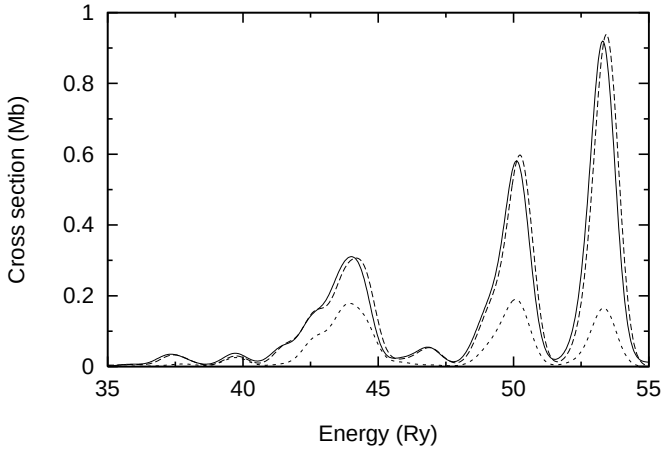

Figure 2. Photorecombination of Fe^{16+} for the LMn ($n = 4$–6) resonances. Short-broken curve, radiation-damped perturbation theory; full curve, undamped perturbation theory; long-broken curve, undamped preconvoluted R-matrix theory—all LS coupling, all this work. All cross sections have been convoluted with a 1 Ryd FWHM Gaussian function.

Ne-like. In figure 2, we present our damped and undamped LS-coupling perturbative results, as well as our undamped preconvoluted R-matrix results, for the LMn ($n = 4$–6) resonances arising in the photorecombination of Fe^{16+} via $2p \rightarrow 3l$ core excitations. The contribution from 2s promotions is small. Again, we note the very close agreement between our undamped perturbative and preconvoluted R-matrix results. The damping factors are now roughly 2, 3 and 4, for $n = 4$, 5 and 6, respectively. This is somewhat of a model calculation since intermediate coupling splits the resonances further apart. (This then limits our undamped preconvoluted R-matrix results to $n = 4$ only.) But it further validates the undamped perturbative approach; which is the main point. The intermediate coupling

perturbative results for this ion (Fe^{16+}) are damped by a factor of 1.85, 2.4 and 4.1 for $n = 3$–5. Again, lower-charge ions are affected by radiation damping; for example, the damping factors for the LMM peak for S^{6+} and Mg^{2+} are 1.43 and 1.39, respectively.

The results that we have presented so far illustrate the sort of damping that can be expected of low-lying photorecombination resonances that arise via $1 \rightarrow 2$ or $2 \rightarrow 3$ core excitations in H-like through Ne-like ions. We can continue on through the periodic table. Moving to $3 \rightarrow 4$ core excitations reduces the distinction between $\Delta n_c = 0$ and $\Delta n_c = 1$ core transitions somewhat, unless we go to higher charge states for example.

Al-like. For Fe^{13+}, the MNn ($n = 4$) peak formed by $3p \rightarrow 4l$ promotions is only damped by a factor of 1.06 but this rises through 1.06, 1.15, 1.34 to 1.73 by $n = 8$.

Ar-like. For Zr^{22+}, the 3p-promoted MNN peak is damped by a factor of 2.7 while that for Fe^{8+} is damped by 1.19.

K-like. For Zr^{21+}, the MNn damping factors for $3d \rightarrow 4l$ promotions are 1.19, 1.79 and 2.0 for $n = 4$–6.

Ni-like. For Zr^{12+}, the 3d-promoted MNN peak is damped by a factor of 1.45 while that for Se^{6+} is damped by 1.19.

These results demonstrate how the radiation damping of low-lying resonances needs to be considered right through to Ni-like ions. One could continue in a similar fashion with $4 \rightarrow 5$ core excitations, say. But this requires a further increase in charge and/or n to maintain a similar level of damping to that we have seen already for $3 \rightarrow 4$ core excitations and so it adds little to our story.

In conclusion, we have demonstrated that perturbation theory provides an accurate description of the effect of radiation damping on R-matrix photorecombination and photoionization resonances and that the effect of damping on low-lying resonances is much more severe, and thus much more widespread, than has been fully appreciated up until now perhaps (see, for example, Pradhan and Zhang 1997). Crucial to this work has been the use of preconvoluted R-matrix photorecombination cross sections. This has enabled us both to find and to fully resolve extremely narrow resonances which contribute significantly to the undamped cross section and which are, probably, the cause of the serious underestimate of undamped cross sections by Zhang and Pradhan (1997) and Pradhan and Zhang (1997) which has led them to seriously underestimate the effect of damping. We note that it has not been possible to include routinely the effect of radiation damping of low-lying resonances in R-matrix calculations until recently, while perturbative calculations would have had no reason to neglect it. The size of the damping effects observed does not necessarily invalidate the large body of undamped R-matrix photorecombination and photoionization data already in existence, such as that generated by the Opacity Project (Seaton 1987). So long as a coarse-enough energy mesh has been used (more precisely, an energy step at least comparable with typical radiative widths) then narrow resonances, that would be completely damped, are not resolved at all in the first place. However, this is a rather hit-and-miss approach—literally so. We emphasize that these findings relate solely to electron–photon transitions. Electron–electron transitions are unaffected and so these findings do not impact upon, for example, the general work of the Iron Project (Hummer *et al* 1993). It should be noted that radiation damping has always been taken into account in perturbative calculations

and it is a non-problem there. From our survey, we see that it is difficult to identify a regime in which it is absolutely safe to carry out an undamped photorecombination and/or photoionization calculation. For many isoelectronic sequences, radiation-damping effects become negligible for a low-enough charge state and principal quantum number, but rapidly become significant as z or n is increased. We can say that it is not safe to assume that radiation damping can be neglected for astrophysical ions, even after excluding the case of H- and He-like ions. It is certainly important for low-n resonances formed via $2 \rightarrow 3$ core excitations, while its importance for $3 \rightarrow 4$ transitions depends on the charge state and resonances of interest. It can also be important for low-temperature photorecombination, via a $2 \rightarrow 2$ non-dipole core excitation, for example. However, we have shown that perturbation theory provides an accurate description of the effect of radiation damping and so can be used to assess the validity of carrying out a *fully resolved* undamped R-matrix calculation for photorecombination and/or photoionization resonances, or it can be used in its own right. Alternatively, one can carry out a full radiation-damped R-matrix calculation as per Robicheaux *et al* (1995) or, if type-I damping dominates, a calculation using the formalism of Bell and Seaton (1985) or the damped form ($\nu \rightarrow \bar{\nu}$) of equation (1) will suffice.

We would like to thank Dr Francis Robicheaux for reading an early version of this manuscript. NRB was supported in part by an EPSRC grant (no GR/K/14346) with the University of Strathclyde and ADP by an EPSRC research studentship.

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