Photorecombination of Highly Charged, Few-Electron Ions: Importance of Radiation Damping and Absence of Resonance Interference

T. W. Gorczyca
Department of Physics, Western Michigan University, Kalamazoo, Michigan 49008-5151

N. R. Badnell
Department of Physics and Applied Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom
(Received 3 March 1997)

We use the radiation damped Breit-Pauli R-matrix method that was introduced by Robicheaux *et al.* [Phys. Rev. A **52**, 1319 (1995)] to study photorecombination of Fe^{24+}. Results are compared to perturbative and experimental results, and agreement is excellent in all cases. It is found that the inclusion of radiation damping is extremely important for this system, whereas resonance interference effects are negligible. These findings are in complete contrast to those of a recent study by Zhang and Pradhan [Phys. Rev. Lett. **78**, 195 (1997)]. [S0031-9007(97)04255-5]

PACS numbers: 34.80.Kw

Photorecombination is the process by which free electrons are accelerated by charged atomic ions and emit photons of sufficient energy such that they are captured by the Coulombic attraction of the ion. This is a cooling mechanism in hot plasmas as well as an important diagnostic [1,2]. Thus, accurate photorecombination cross sections are required for a wide variety of ions for the modeling of these plasmas, whether in fusion [1] or astrophysics [2] research. The bulk of the required cross sections must be obtained from numerical calculations since there is only limited experimental data available [3]. The most demanding aspect of any calculation is the treatment of the dominant resonant process of dielectronic recombination (DR), whereby the incident electron is captured by the ion into a doubly excited resonance state, followed by radiative stabilization via the spontaneous emission of a photon. This presents a great challenge to atomic theorists. Since there are an infinite number of Rydberg states converging to each excited state of the target ion, an efficient method for computing and mapping out the rich spectrum of DR resonances is needed. In addition, the lifetimes of these resonances are affected by the interaction between the (zero-photon) radiation field and the scattering (and target) electrons; this becomes more important as the residual charge on the ion increases. The resultant resonance profile is reduced and broadened, a phenomenon known as radiation damping [4,5]. It is also possible that members of neighboring Rydberg series may interact with each other, giving rise to resonance interference phenomena, further complicating the theoretical treatment.

The purpose of this Letter is to compute Breit-Pauli R-matrix [6,7] photorecombination cross sections for Fe^{24+}, both with and without radiation damping, so as to assess the degree of damping effects, and also to compare with perturbative results so as to assess the degree of interfering resonance effects. While we find the former effects to be very large, the latter effects are undetectable. This is in complete contrast to the findings of a recent Letter [8].

There are two commonly used numerical approaches for the calculation of DR cross sections: (1) perturbative methods [9,10]; and (2) nonperturbative methods that solve the close-coupling equations, and use the resulting scattering matrices, together with appropriate radiative interaction potentials, to predict photorecombination probabilities. The widely accepted most efficient and accurate approach for solving the close-coupling equations is the R-matrix method [11], which can be extended to compute photorecombination [12,13]. The advantages of perturbative methods are that (1) the computed resonance positions, autoionization widths, and radiative widths are used as input into an analytic formula that economically yields the detailed DR spectra at any level of resolution desired, and (2) the inclusion of radiation damping effects is straightforward. The main disadvantage of lowest-order perturbative methods compared to the R-matrix method is that higher-order effects such as quantum interference between resonance processes is not usually included. While it is possible to extend perturbative methods to higher orders to incorporate these effects, a general algorithm for treating the interaction of two or more Rydberg series does not exist presently. The R-matrix method, on the other hand, incorporates these interference effects to all orders.

The main difficulty with one implementation of photorecombination within the R-matrix method, namely, the calculation of photoionization cross sections (to obtain the photorecombination cross sections through the detailed balance relationship [12]), is that the lifetimes of the resonances are treated in the absence of radiation damping. This does not present a problem for low-charged ions since the effects of radiation damping are insignificant for low-lying resonances. Indeed, there have been numerous Breit-Pauli R-matrix calculations for the photoionization of neutral atoms [14]. It is well known, however, that as the ionic charge is increased, radiation damping for $\Delta n > 0$ DR rapidly becomes more important. As demonstrated in the case of the photoionization of Fe^{24+} [15], this effect caused a factor of 6 reduction in the peak resonance cross section compared to undamped results. Recently, Robicheaux *et al.* [13] presented a new approach, based on the use of a radiative optical potential, for treating photorecombination *with* radiation damping within any close-coupling method, and, in particular, the R-matrix method. The approach was subsequently applied to the treatment of photorecombination of Mo^{41+} [16] to show that, similar to the study on the photoionization of Fe^{24+}, this method yielded damped resonance cross section peaks which were an order of magnitude smaller than results obtained in the absence of the radiative optical potential.

A recent Letter by Zhang and Pradhan [8] described the use of the Breit-Pauli R-matrix inverse-photoionization method *without* radiation damping to treat photorecombination of Fe^{24+} and Ar^{13+}. The photorecombination treated in Ar^{13+} proceeds via $\Delta n = 0$ DR, so that radiation damping is not significant for low n, although we find it to be a noticeable effect. Their R-matrix results, compared to experiment, were of the same level of accuracy as separate perturbative results [17], which is in line with the findings of a recent Breit-Pauli R-matrix and perturbative study for the photorecombination of Ar^{15+} [18]. In the case of Fe^{24+}, on the other hand, the dominant DR mechanism proceeds via a $\Delta n > 0$ transition. While Zhang and Pradhan made no quantitative comparison with experiment, they did compare to perturbative results [19] and found that their R-matrix convoluted cross sections were only about two-thirds of the perturbative ones for the lowest resonances (KLL), which is surprising. They also suggested that this difference was due to resonance interference effects and noted that the tails of the Lorentzian profiles of neighboring resonances were indeed overlapping, when viewed on an appropriate scale. In view of previous studies on damped vs undamped photorecombination of Fe^{25+} [15] and Mo^{41+} [16], a further reduction by about a factor of 6 should be expected if these inverse-photoionization calculations were performed *with* radiation damping. Thus, resonance interference effects would seemingly cause a reduction in the computed photorecombination cross sections by *roughly an order of magnitude,* which would be highly surprising [20]. To summarize, Zhang and Pradhan [8] stated in effect that their results indicated that radiation damping effects, which they did not include in their R-matrix calculations, were not particularly significant for Fe^{24+} but that interfering resonance effects were.

We now investigate radiation damping and interfering resonance effects. The R-matrix method that we used for the damped calculations is based on the radiative optical potential treatment of photorecombination due to Robicheaux *et al.* [13]. The implementation of this method was further modified so as to compute *partial* photorecombination cross sections to final states contained within the R-matrix box, from the appropriate dipole matrices, both with and without the inclusion of the optical potential in the Hamiltonian; the latter is precisely equivalent to the inverse-photoionization treatment of photorecombination [8,12]. The Breit-Pauli distorted-wave (BPDW) perturbative results were obtained from the program AUTOSTRUCTURE [9]. All of our R-matrix and perturbative calculations used identical atomic orbitals and identical configurations $1snl$ ($nl = \{1s, 2s, 2p, 3s, 3p\}$) to describe the lowest 13 target levels of Fe^{24+}.

We first show a comparison between our nondamped and damped Breit-Pauli R-matrix results for the KLL ($1s2l2l'$) resonances in Fig. 1(a). We plot the collision strength, Ω_i, which is related to the recombination cross section, σ_i, via $\Omega_i = \omega_i E_i \sigma_i / \pi a_0^2$, where ω_i is the statistical weight of the initial level i and E_i is the energy (in Rydbergs) of the electron incident on i. We choose the vertical scale such that the broad tails of the Lorentzian profiles can be seen. The two are nearly identical on this scale. On the other hand, if we plot the collision strengths on a scale where the (damped) maximum is visible, then differences are quite noticeable [see Fig. 1(b)]; the undamped collision strengths actually peak at a much higher value than the damped ones. This choice of vertical scale also illustrates that the resonance widths, which are roughly comparable to the width of the figure lines for this horizontal scale, are obviously much less than the energy separation of any two resonances, and so these resonances cannot be considered "overlapping and interfering." In Fig. 1(c), we magnify the region of one of the narrower resonances ($1s2p^2\,{}^2P_{3/2}$, which cannot autoionize in LS coupling) in order to see that the effect of radiation damping is to reduce the peak collision strength by almost 4 orders of magnitude. The convoluted collision strengths for our two sets of R-matrix

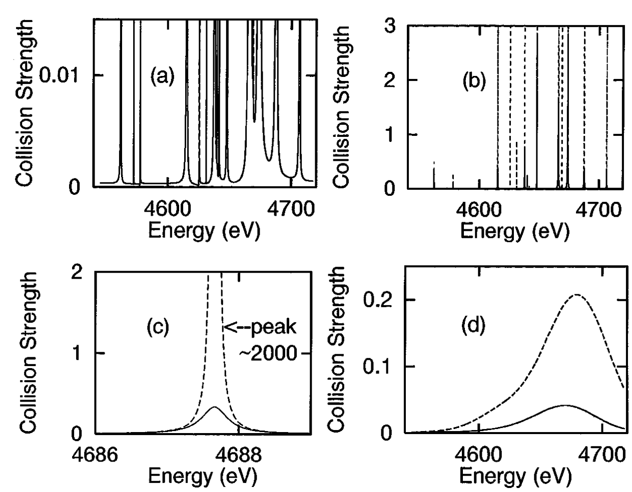

FIG. 1. Photorecombination collision strengths for the KLL resonances of Fe^{24+}: Dashed line, inverse-photoionization method (without damping); solid line, radiative optical potential method (equivalent to inverse-photoionization method with damping); (a), (b), and (c) are unconvoluted, (d) is convoluted with a 50 eV FWHM Gaussian.

results (damped and undamped) are shown in Fig. 1(d), showing roughly a factor of 7 damping. We next show a comparison between damped R-matrix and (damped) perturbative Breit-Pauli results in Fig. 2, both with and without convolution, in order to see that the positions, shapes, and convoluted collision strengths are in excellent agreement. This clearly demonstrates that interfering resonance effects are negligible for these KLL resonances. It has been suggested [8] that the perturbative method cannot yield detailed resonance structure; as we see, this is not the case. Finally, we show our photorecombination collision strengths for the entire $1s2lnl'$ series in Fig. 3. The agreement between our *damped* R-matrix and perturbative results is excellent across the entire energy range. Caution should be exercised in comparing these collision strengths with Fig. 1(b) of Zhang and Pradhan [8]. Despite apparently identical definitions of the collision strength in terms of the cross section, if we convert their collision strength to a cross section and convolute with a Maxwellian distribution, we do not recover the rate coefficients in their Table I. There appears to be a factor of 2 difference in the definition of collision strength used in practice. Also, it is not clear whether their collision strength is for total recombination or just K_α recombination.

In Table I, we make quantitative comparisons between our results, the experimental results of Beiersdorfer *et al.* [21], and the R-matrix results of Zhang and Pradhan [8]. We note the good agreement between our perturbative and R-matrix results, both damped and undamped. However, we obtain a large damping factor (8–800 for $KLn, n = 2$–6, for our BPDW results). While the results of Zhang and Pradhan [8] are generally larger than our damped results, they are not comparable with our undamped results. In order to try and shed light on the situation, we have carried out undamped calculations along the lines of Ref. [8], i.e., by using the photoionization code STGBF and applying detailed balance. Only by using a coarse energy mesh (a total of $\sim$10 000 points), more suited to electron-impact excitation, do we obtain results similar to those of Zhang and Pradhan [8], who give no information regarding their energy mesh. We find that an extremely fine energy mesh is required to find, let alone resolve, a myriad of extremely narrow resonances (of width $\sim 10^{-8} z^2$ Ry) which contribute significantly to the undamped cross section. Indeed, only by using our perturbative results as a guide was it possible to search out and delineate these resonances to obtain the undamped R-matrix results, for KLL and KLM only. These narrow resonances contribute little to the damped results, and so their omission by an undamped calculation can lead to a result that vaguely resembles an undamped result, assuming that all of the broad resonances which are much less affected by damping are included still. The importance of comparing the radiative width to the *smallest* autoionizing width for photorecombination, to assess the role of damping, as opposed to the *largest* autoionizing width, which is relevant for electron-impact excitation, is discussed in detail in Ref. [16]. Experimental results summed over all final states only exist for the KLL resonances [21]. The experimental integrated cross sections were normalized by Beiersdorfer *et al.* [21] using a well established theoretical radiative recombination cross section. The estimated experimental uncertainty is 20% [21]. We note the excellent agreement between our damped R-matrix results and experiment for the KLL resonances.

Finally, in Table II, we compare our perturbative results with the experimental results of Beiersdorfer *et al.* [22] for K_α recombination. This is the recombination arising from inner-electron stabilization only. The experimental integrated cross sections were normalized by Beiersdorfer *et al.* [22] using a well established theoretical excitation

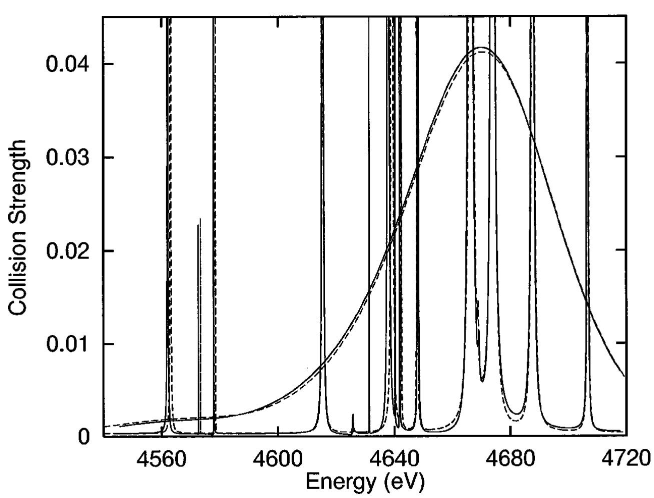

FIG. 2. Photorecombination collision strengths for the KLL resonances of Fe^{24+}: Solid line, R-matrix results; dashed line, perturbative results; convoluted results (with a 50 eV FWHM Gaussian) are also shown.

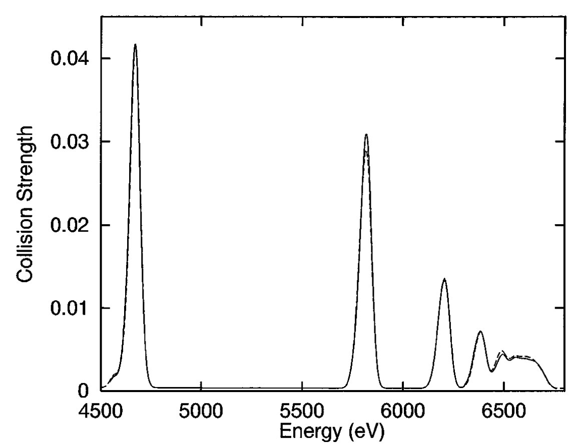

FIG. 3. Photorecombination collision strengths for the KLn $(2 \leq n \rightarrow \infty)$ resonances of Fe^{24+}: Solid line, R-matrix results; dashed line, perturbative results. Both are convoluted with a 50 eV FWHM Gaussian.

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

KLn	Undamped BPDW[b]	Undamped BPRM[b]	Damped BPDW[b]	Damped BPRM[b]	BPRM[c]
KLL[a]	18.9	17.5	2.417	2.455	1.784
KLM	30.2	28.2	1.033	1.117	1.147
KLN	40.9		0.380	0.377	0.529
KLO	57.5		0.180	0.179	0.307
KLP	78.5		0.100	0.096	0.223
$KLn \geq 7$			0.230	0.219	0.762

[a]Experimental result = 2.48, Beiersdorfer *et al.* [21].
[b]This work.
[c]Zhang and Pradhan [8].

cross section. We see that the agreement between theory and experiment is excellent—within the estimated experimental uncertainty (of 15%), except for the small *KLO* peak which was barely resolvable, in the experiment, from the higher-energy peaks [22]. By comparing with Table I, we see that the K_α recombination dominates the total recombination and so the experiment clearly differentiates between our results and those of Zhang and Pradhan [8].

In conclusion, we find that the effect of radiation damping in the photorecombination of Fe^{24+} is to reduce significantly the convoluted collision strengths, while resonance interference effects are negligible. Furthermore, our results are in excellent agreement with experiment. There are two important implications of these findings for the theoretical treatment of photorecombination in highly charged few-electron ions. First, properly performed photorecombination calculations using the close-coupling method without radiation damping will predict cross sections perhaps 1 or 2 orders of magnitude larger than the correct damped ones. The size of this effect means that, more generally, undamped R-matrix calculations for photorecombination and/or photoionization resonances should only be performed after a careful assessment of the effect of damping. Second, as in the findings of an earlier study [20], it remains the case that detection of interfering resonance effects in photorecombination will be extremely difficult. Our verification of the standard perturbative approach, which was called into question by the inexplicable findings of Zhang and Pradhan [8], is extremely important for spectroscopic modelers of laboratory and astrophysical non-LTE plasmas, who make widespread use of perturbative DR data.

TABLE II. K_α partial photorecombination rate coefficients for Fe^{24+} at $T = 2$ keV (10^{-13} cm^3 s^{-1}).

KLn	Experiment[a]	BPDW[b]
KLM	0.73	0.695
KLN	0.22	0.256
KLO	0.09	0.124
$KLn \geq 6$	0.21	0.236

[a]Beiersdorfer *et al.* [22].
[b]This work.

N. R. B. was supported in part by a U.K. EPSRC contract (No. GR/K/14346) with the University of Strathclyde.

[1] H. P. Summers, Adv. At. Mol. Opt. Phys. **33**, 275 (1994).
[2] H. E. Mason and B. C. Monsignori-Fossi, Astron. Astrophys. Rev. **6**, 123 (1994).
[3] G. H. Dunn, Nucl. Fusion Suppl. **2**, 25 (1992).
[4] P. C. W. Davies and M. J. Seaton, J. Phys. B **2**, 757 (1969).
[5] R. H. Bell and M. J. Seaton, J. Phys. B **18**, 1589 (1985).
[6] N. S. Scott and K. T. Taylor, Comput. Phys. Commun. **25**, 347 (1982).
[7] K. A. Berrington, W. B. Eissner, and P. H. Norrington, Comput. Phys. Commun. **92**, 290 (1995).
[8] H. L. Zhang and A. K. Pradhan, Phys. Rev. Lett. **78**, 195 (1997).
[9] N. R. Badnell, J. Phys. B **19**, 3827 (1986).
[10] M. H. Chen, Phys. Rev. A **31**, 1449 (1985).
[11] P. G. Burke and K. A. Berrington, *Atomic and Molecular Processes: An R-matrix Approach* (IOP Publishing, Bristol, 1993).
[12] S. N. Nahar and A. K. Pradhan, Phys. Rev. A **49**, 1816 (1994).
[13] F. Robicheaux, T. W. Gorczyca, M. S. Pindzola, and N. R. Badnell, Phys. Rev. A **52**, 1319 (1995).
[14] M. Aymar, C. H. Greene, and E. Luc-Koenig, Rev. Mod. Phys. **68**, 1015 (1996).
[15] K. Sakimoto, M. Terao, and K. A. Berrington, Phys. Rev. A **42**, 291 (1990).
[16] T. W. Gorczyca and N. R. Badnell, J. Phys. B **29**, L283 (1996).
[17] D. R. DeWitt, R. Schuch, W. Zong, S. Asp, C. Biedermann, M. H. Chen, and N. R. Badnell, Phys. Rev. A **53**, 2327 (1996).
[18] T. W. Gorczyca, F. Robicheaux, M. S. Pindzola, and N. R. Badnell, Phys. Rev. A **54**, 2107 (1996).
[19] D. H. Sampson and H. L. Zhang, J. Quant. Spectrosc. Radiat. Transfer **54**, 345 (1995).
[20] M. S. Pindzola, N. R. Badnell, and D. C. Griffin, Phys. Rev. A **46**, 5725 (1992).
[21] P. Beiersdorfer, T. W. Phillips, K. L. Wong, R. E. Marrs, and D. A. Vogel, Phys. Rev. A **46**, 3812 (1992).
[22] P. Beiersdorfer, M. B. Schneider, M. Bitter, and S. von Goeler, Rev. Sci. Instrum. **63**, 5029 (1992).