Resonance contributions to the electron-impact ionization of few-electron highly charged ions

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(Received 28 August 1992)

We present results for the electron-impact ionization of Li-like, Be-like, and B-like Fe, Kr, and Xe ions. We have included the contributions from direct ionization, excitation autoionization, and dielectronic-capture double autoionization in our calculations. We discuss isonuclear and isoelectronic trends for the various contributions, focusing on the resonance contributions in particular.

PACS number(s): 34.80.Kw

I. INTRODUCTION

Highly charged heavy ions are currently the focus of much attention at experimental facilities such as the Test Storage Ring at the Heidelberg, the Experimental Storage Ring at Gesellschaft für Schwerionenforschung in Darmstadt, and the Electron Beam Ion Trap at LLNL. They are also present in magnetic fusion plasmas: Fe is an ever-present impurity while Kr and Xe are introduced for diagnositic purposes. Thus, there is great interest in theoretical studies of electron collisions with highly charged ions. In this paper we focus on ionization. Both the direct ionization process and the important indirect process of excitation autoionization have been studied extensively in the past few years—both experimentally [1] and theoretically [2]. The current interest lies with the additional indirect process of dielectronic-capture double autoionization. The Li-like sequence has been studied extensively at low charge states ($Z<10$). The high-resolution crossed-beam measurements of Hofmann *et al.* [3] are in good agreement with the theoretical predictions of the close-coupling approximation [4] and of the independent-processes isolated-resonance approximation [5]. As the charge on the ion increases the resonances become more prominent (initially) since they scale as Z^{-3} compared to the Z^{-4} scaling of the excitation-autoionization cross section. Comparisons of theory [6,7] and experiment [8,9] for electron-impact ionization of the Na-like ions Fe^{15+} and Xe^{43+} showed good agreement, but the sizes of the predicted resonances and the energy resolution and uncertainties in the experimental cross section were such that no resonances were observed. Recently, Chen and Reed [10(a)] showed that resonance contributions may persist strongly for Li-like ions at high-charge states (e.g., Xe^{51+}) where initially one might think that they would be eliminated by radiation damping. In this paper we present the results of calculations for the electron-impact ionization of Li-like, Be-like, and B-like Fe, Kr, and Xe ions, focusing on energies around the dominant group of resonances—the *KMM*. The Li-like results are included both for isonuclear comparisons and because we find the resonance contributions to be substantially smaller than those of Chen and Reed [10(a)]. The layout of the paper is as follows. We present a brief description of the required theory in Sec. II and its application to the problem at hand in Sec. III. We present and discuss our results in Sec. IV and provide conclusions in Sec. V.

II. THEORY

In the independent-processes approximation, the total ionization cross section from the ground level g of an ion, $\sigma(g;\mathrm{tot})$, is given by the sum of the direct plus excitation-autoionization and dielectronic-capture double-autoionization contributions. Thus,

$$\sigma(g;\mathrm{tot})=\sigma_d(g)+\frac{\sum_i \sigma_x(g\to i)\sum_k A_a(i\to k)}{\sum_k A_a(i\to k)+\sum_f A_r(i\to f)}+\frac{\sum_j \bar{\sigma}_c(g\to j)\sum_i A_a(j\to i)\sum_k A_a(i\to k)}{\left\{\sum_i A_a(j\to i)+\sum_f A_r(j\to f)\right\}\left\{\sum_k A_a(i\to k)+\sum_f A_r(i\to f)\right\}}\ , \quad (1)$$

where $\sigma_d(g)$ is the direct-ionization cross section, $\sigma_x(g\to i)$ is the excitation cross section for the autoionizing level i, and $\bar{\sigma}_c(g\to j)$ is the energy-averaged dielectronic capture cross section for the isolated doubly autoionizing level j. A_a and A_r denote autoionization and radiative rates, respectively. In this independent-processes approximation we see that the excitation cross sections get multiplied by a single branching ratio or Auger yield, and the dielectronic-capture cross sections by two sequential Auger yields. Through detailed balance we have

$$\bar{\sigma}_c(g\to j)=\frac{(2\pi a_0 I_H)^2}{E\Delta E}\frac{\omega(j)}{2\omega(g)}\tau_0 A_a(j\to g)\ , \quad (2)$$

where $\omega(j)$ is the statistical weight of the captured level j

and $\omega(g)$ is the statistical weight of the ground level. E is the energy of the electron incident on the ground level, ΔE the bin width, and $(2\pi a_0)^2\tau_0 = 2.6741\times 10^{-32}$ cm^2 s. These isolated-resonance and independent-processes approximations for ionization are analogous to those used for recombination. For the computationally intensive dielectronic-capture double-autoionization contribution, it enables us to carry over much of the work originally developed for recombination. The close-coupling approximation, as applied to ionization, does allow for overlapping resonances and for interference between the excitation-autoionization and dielectronic-capture double-autoionization contributions, but it does not allow for radiation damping. However, these overlapping and interfering effects are generally small for highly charged ions but, as we shall see, the radiation damping effects are by no means negligible. The differences that arise on using a distorted-wave versus a close-coupling approximation for the $(N+1)$-electron wave function are also small for highly charged ions.

III. APPLICATION

Our first application of the theory of Sec. II is to the ionization of highly charged Li-like, Be-like, and B-like ions since they have a relatively simple atomic structure and are of current experimental interest. Eventually, we hope to employ the same techniques to more complex systems. Because of the high-charge states involved semirelativistic distorted-wave functions [11] were used in all of the calculations. The direct ionization cross sections were calculated in the configuration-average approximation using the first Born approximation, a triple partial-wave expansion, and the maximum interference approximation [12]. The excitation autoionization [12,13] and dielectronic-capture double-autoionization [14] cross sections were calculated in explicit level-to-level configuration-mixing and intermediate coupling approximations which fully allow for radiation damping. Our main interest is the energy region in which resonances may be important. Consequently, we include only L-shell direct ionization and KL-excitation-autoionization contributions; in any case we find the KM-excitation-autoionization contribution to be very small. The direct-ionization calculations used a single-configuration approximation since configuration-mixing effects are expected to be very small; for highly charged Be-like ions they are only a 1% effect [15]. Configuration mixing was taken into account in the excitation-autoionization calculations. The configurations and transitions that were included are detailed below:

$$
\begin{array}{l}
1s^22s + e^- \rightarrow 1s2l2l' + e^- \rightarrow 1s^2 + 2e^- \quad \text{(Li-like)} \\
\qquad\qquad\qquad \downarrow \\
\qquad\qquad\qquad 1s^22l + h\nu \, ,
\end{array}
$$

$$
\begin{array}{l}
\left.\begin{matrix} 1s^22s^2 \\ 1s^22p^2 \end{matrix}\right\} + e^- \rightarrow \left.\begin{matrix} 1s2s^22p \\ 1s2p^3 \end{matrix}\right\} + e^- \rightarrow 1s^22l + 2e^- \quad \text{(Be-like)} \\
\qquad\qquad\qquad \downarrow \\
\qquad\qquad\qquad \left.\begin{matrix} 1s^22s^2 \\ 1s^22p^2 \end{matrix}\right\} + h\nu \, ,
\end{array}
$$

$$
\begin{array}{l}
\left.\begin{matrix} 1s^22s^22p \\ 1s^22p^3 \end{matrix}\right\} + e^- \rightarrow \left.\begin{matrix} 1s2s^22p^2 \\ 1s2p^4 \end{matrix}\right\} + e^- \rightarrow 1s^22l2l' + 2e^- \quad \text{(B-like)} \\
\qquad\qquad\qquad \downarrow \\
\qquad\qquad\qquad \left.\begin{matrix} 1s^22s^22p \\ 1s^22p^3 \end{matrix}\right\} + h\nu \, .
\end{array}
$$

The dominant contribution from dielectronic-capture double autoionization is from the KMn series and in particular the KMM resonances. The contribution from the KLn series is small, since the lowest-n values are energetically inaccessible in highly charged ions, and falls off rapidly with n ($\sim n^{-3}$) [10(a)]. Thus, we focus on the KMM resonances in our isonuclear and isoelectronic studies. Below, we give details of the particular transitions that we included for each isoelectronic sequence:

$$
\begin{array}{l}
\left.\begin{matrix} 1s^22s \\ 1s^22p \\ 1s^23l \end{matrix}\right\} + e^- \rightleftarrows \left\{\begin{matrix} 1s2s3l3l' \\ 1s2p3l3l' \end{matrix}\right\} \rightarrow 1s2l2l' + e^- \rightarrow \quad 1s^2 + 2e^- \quad \text{(Li-like)} \\
\qquad\qquad\qquad \downarrow \qquad\qquad\qquad\qquad\qquad\qquad\qquad \downarrow \\
\qquad\qquad\qquad \left.\begin{matrix} 1s^22l3l \\ 1s^23l3l' \\ 1s2l2l'3l'' \end{matrix}\right\} + h\nu \quad 1s^22l + h\nu \, ,
\end{array}
$$

$$\left.\begin{array}{l} 1s^22s^2 \\ 1s^22p^2 \\ 1s^22l3l' \end{array}\right\} + e^- \rightleftarrows \begin{array}{l} \left\{\begin{array}{l} 1s2s^23l3l' \\ 1s2p^23l3l' \end{array}\right\} \\ \downarrow \\ \left.\begin{array}{l} 1s^22s^23l \\ 1s2s^22p3l \\ 1s^22l3l'3l'' \\ 1s^22p^23l \\ 1s2s2p^23l \\ 1s2p^33l \end{array}\right\} + h\nu \end{array} \begin{array}{l} \rightarrow \\ \\ \\ \end{array} \begin{array}{l} \left.\begin{array}{l} 1s^23l3l' \\ 1s2s^22p \\ 1s2p^3 \end{array}\right\} + e^- \rightarrow 1s^22l + 2e^- \quad (\text{Be-like}) \\ \downarrow \\ \left.\begin{array}{l} 1s^22s^2 \\ 1s^22p^2 \\ 1s^22l3l' \end{array}\right\} + h\nu \, , \end{array}$$

$$\left.\begin{array}{l} 1s^22s^22p \\ 1s^22s^23l \\ 1s^22s2p3l \end{array}\right\} + e^- \rightleftarrows \begin{array}{l} 1s2s^22p3l3l' \\ \downarrow \\ \left.\begin{array}{l} 1s^22s^23l3l' \\ 1s^22s^22p3l \\ 1s2s^22p^23l \end{array}\right\} + h\nu \end{array} \begin{array}{l} \rightarrow \\ \\ \\ \end{array} \begin{array}{l} \left.\begin{array}{l} 1s^22l''3l3l' \\ 1s2s^22p^2 \end{array}\right\} + e^- \rightarrow 1s^22l2l' + 2e^- \quad (\text{B-like}) \\ \downarrow \\ \left.\begin{array}{l} 1s^22l2l'3l'' \\ 1s^22s^22p \end{array}\right\} + h\nu \, . \end{array}$$

In the case of the Li-like ions, the $1s2p3l3l'$ configurations do not contribute directly to ionization. They and their associated electron and photon continua were included to investigate the effect of configuration mixing on the first autoionization step. Configuration mixing at the second autoionizing step ($1s2s^2+1s2p^2$) must always be included [10(a)]. Similarly, the $1s2p^23l3l'$ and $1s2p^3$ configurations were included to allow for configuration mixing in the Be-like problem. By the time we reach the B-like sequence, configuration mixing of this form ($2s^22p+2p^3$) is not expected to be important because the $2p^3$ configuration does not open up any new radiative channels for the $2s^22p$ configuration.

IV. RESULTS

We present our results for the electron-impact ionization of Fe, Kr, and Xe ions in Figs. 1–3; within each figure there are results for the Li-, Be-, and B-like ions. The cross sections have been convoluted with a 1.5-Ry Gaussian function to facilitate study of the resonance contributions. We discuss first the behavior of the *KMM* dielectronic-capture double-autoionization cross sections. In the absence of radiation damping, the *KMM* integrated cross section varies slowly along an isonuclear sequence since the active capture in each case is given by $1s^2+e^- \rightarrow 1s3l3l'$ and the double Auger yield is close to unity since the $3 \rightarrow 2$ autoionization rates dominate over the $3 \rightarrow 1$. For example, the *KMM* cross section for Fe^{22+} is 12% smaller than that for Fe^{23+} and that for Fe^{21+} is 13% smaller than that for Fe^{22+}, with the radiation damping switched off. Furthermore, configuration mixing has little quantitative effect; it merely redistributes the cross section amongst the autoionizing levels. Finally, the $1/E$ dependence dominates the scaling along an isoelectronic sequence.

When radiation damping is included, results within an isonuclear sequence can change dramatically from one ion to the next. For Fe, the ratio of Be-like to Li-like *KMM* cross sections is 1.92 and B-like to Li-like 1.28; for Xe, the ratios are 3.3 and 1.45. For Li-like ions, most of

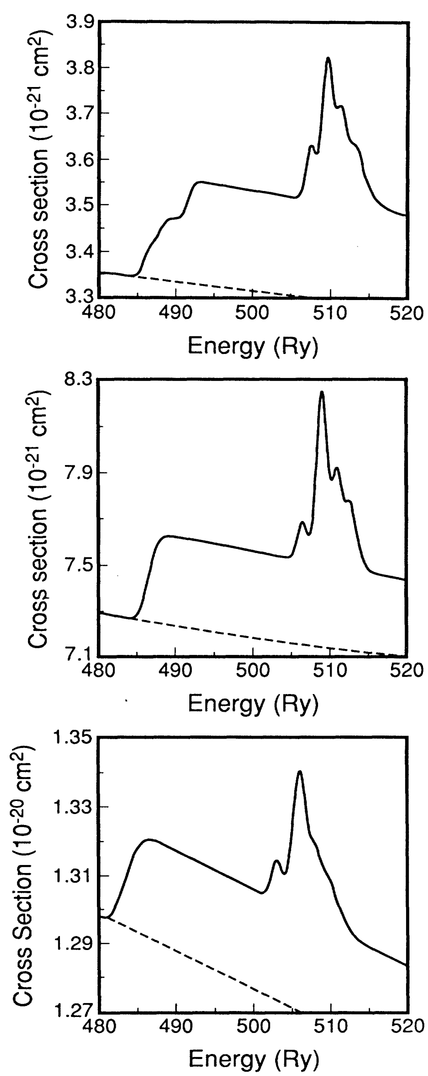

FIG. 1. Electron-impact ionization of Fe ions. Top, Fe^{23+}; middle, Fe^{22+}; bottom, Fe^{21+}.

the radiation damping is on the second autoionizing step and configuration mixing of the $1s2s^2\,{}^2S_0$ and $1s2p^2\,{}^2S_0$ levels can reduce the $1s2s^2\,{}^2S_0$ Auger yield significantly, by a factor of 2 for Xe^{51+}. Configuration mixing in the first autoionizing step (due to $1s2p3l3l'$) causes a 20–30 % reduction. The overall effect is that radiation damping reduces the *KMM* Li-like cross sections by a factor of 3.0, 5.6, and 24 for Fe, Kr, and Xe, respectively. For Be-like and B-like ions, the presence of core $+3l3l'$ configurations in the second autoionizing step reduces the effect of radiation damping compared to Li-like ions, although in the B-like case this is offset somewhat by the increased damping in the first autoionizing step due to the $2p \rightarrow 1s$ radiation. Also, for B-like ions, all levels of the $1s2s^22p^2$ configuration have a direct $E1$ transition to a level of the $1s^22s^22p$ configuration. The net result is that the B-like *KMM* cross sections are not reduced as strongly as the Li-like ones, but the factors are still 1.8, 5.2, and 14.5 for Fe, Kr, and Xe, respectively. All of the B-like results presented here have been averaged over the $J=\frac{1}{2}$ and $\frac{3}{2}$ levels of the ground configuration. Cross sections from the $J=\frac{3}{2}$ level are up to 30% larger than those from the $J=\frac{1}{2}$ level. Radiation damping effects are further reduced for Be-like ions since the $1s2s^22p\ {}^3P_{0,2}$ levels only radiate through mixing and they do not mix as strongly with the $1s2p^3\,{}^3P_{0,2}$ levels as in the analogous case for Li-like ions. For Xe^{50+}, the $1s2s^22p\ {}^3P_{0,2}$ Auger yields are 0.96 and 0.65 compared to 0.50 for the $1s2s^2\,{}^2S_0$ level in Xe^{51+}. This mixing reduces the Be-like results by 2–20 %. Similarly, $2s^2+2p^2$ mixing in the first autoionizing step causes a 1–20 % reduction in the *KMM* cross sections for Fe-Xe. Thus, Be-like results are only reduced by radiation damping by a factor of 1.4, 2.7, and 5.0 for Fe, Kr, and Xe, respectively. The Be-like reso-

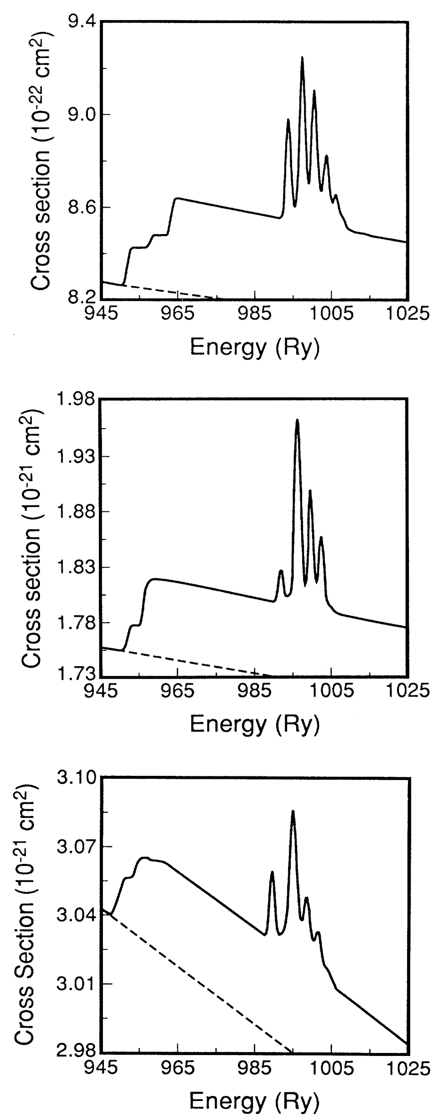

FIG. 2. Electron-impact ionization of Kr ions. Top, Kr^{33+}; middle, Kr^{32+}; bottom, Kr^{31+}.

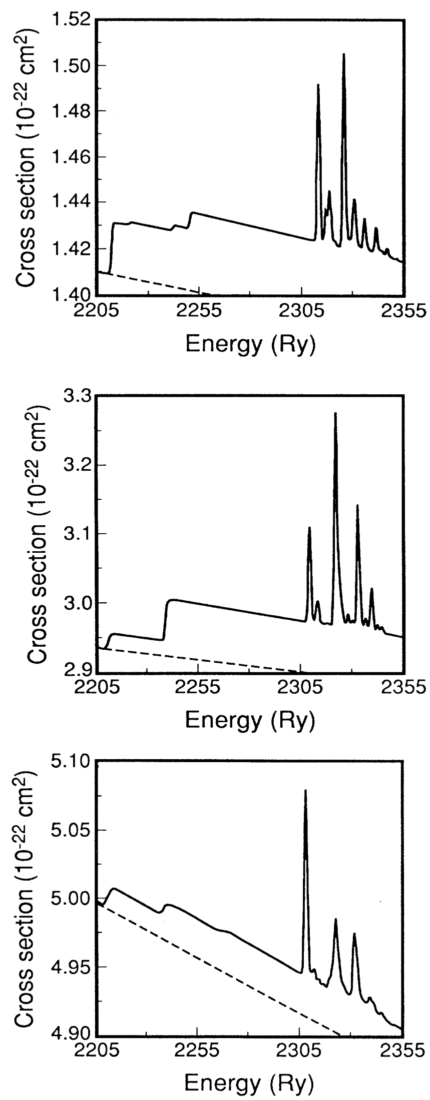

FIG. 3. Electron-impact ionization of Xe ions. Top, Xe^{51+}; middle, Xe^{50+}; bottom, Xe^{49+}.

nance cross sections persist more strongly at high-charge states than the Li-like or B-like ones, the Xe^{50+} results being a factor of 3.3 greater than the Xe^{51+} results and a factor of 2.3 greater than the Xe^{49+} results.

The excitation-autoionization contribution shows some of the same isonuclear and isoelectronic scaling behavior as the dielectronic-capture double-autoionization contribution. Indeed, the set of autoionizing states formed by inner-shell excitation is the same set that results from dielectronic capture followed by a single autoionization. The decay of this set of autoionizing states was discussed in the preceding paragraph. The excitation-autoionization cross sections vary slowly along an isonuclear sequence in the absence of radiation damping. The Fe^{22+} results are 13% smaller than the Fe^{23+} results and the Fe^{21+} results are 13% smaller than the Fe^{22+} results. Again, the Be-like sequence is less sensitive to radiation damping than the Li-like and B-like sequences. The Be-like results are reduced by a factor of 1.7, 2.5, and 3.8 for Fe, Kr, and Xe, respectively, while the Li-like and B-like reduction factors are 3.4, 4.8, and 11.1, and 1.8, 3.5, and 8.5, respectively. There is a negligible difference between the single configuration and multiconfiguration results, for both Be-like and B-like ions, and between the $j=\frac{1}{2}$ and $j=\frac{3}{2}$ initial level results for B-like ions. Just below the excitation-autoionization thresholds, some small amount of fill-in should be expected due to the *KLn* series of resonances which were omitted from our calculations.

The absolute values of the dielectronic-capture double-autoionization cross sections for Be-like ions are much greater than for the Li-like and B-like ions. But, the direct ionization cross section increases by just over a factor of 2 on going from Li-like to Be-like ions (due to the $2s$ occupancy) and by nearly another factor of 2 on going to B-like ions. The sharper falloff of the direct ionization cross section with energy for B-like ions is due to the more weakly bound $2p$-orbital contribution. The Be-like excitation-autoionization cross sections are also a factor of 2–3 greater than the Li-like or B-like ones. This means that, relative to the slowly varying "background" (direct plus excitation-autoionization contributions) the Be-like resonance contributions are only a little larger than the Li-like ones, but both are still relatively larger than the B-like contributions, substantially so in fact. It is this relative behavior which is probably of more relevance to experiment than the absolute values, given that the cross sections differ by no more than a factor of 5 along an isonuclear sequence.

Recently, Chen and Reed [10(a)] published results similar to ours for the Li-like ions. Our direct and excitation-autoionization results are smaller than theirs [10(a)] by up to 20%. However, our results for the *KMM* resonances are smaller by a factor of 1.5, 2.0, and 3.5 for Fe^{23+}, Kr^{33+}, and Xe^{51+}, respectively. Only a small part of the difference is due to the additional configuration mixing that we included in our calculations (see above). A detailed comparison of the two sets of results by Chen [10(b)] and one of us (N.R.B.) revealed that the $1s2s2p\ {}^4P_{5/2}$ Auger yield used in the evaluation of the double Auger yields only was accidentally taken to be unity by Chen and Reed [10(a)]. If we take our $1s2s2p\ {}^4P_{5/2}$ Auger yield to be unity, we can reproduce the *KMM* cross sections of Chen and Reed [10(a)] to within 20%, the same level of accord as noted previously for the direct and excitation-autoionization contributions. The remaining differences may be due in part to our use of semirelativistic wave functions compared to the fully relativistic ones used by Chen and Reed [10(a)] and/or a different choice of phase in the case of the direct ionization calculations.

V. CONCLUSION

We have carried out isonuclear and isoelectronic studies of the electron-impact ionization of highly charged Fe, Kr, and Xe ions, focusing on the *KMM* resonances in particular. We have found that resonance contributions for the Li-like sequence are much smaller than previously thought. But, we also found that resonance contributions for the Be-like sequence are not as affected by radiation damping as for the Li-like sequence, or indeed the B-like sequence. A similar statement can be made about the excitation-autoionization contributions as well. The size of the resonance contributions relative to the background for Li-like and particularly Be-like ions may make them more preferable sequences for a high-resolution experimental search for resonance contributions to ionization than the B-like and, by implication, more complex second-row ionic sequences.

ACKNOWLEDGMENTS

One of us (N.R.B.) would like to thank Dr. M. H. Chen for some helpful discussions. This work was supported by the U.S. Department of Energy, Office of Fusion Energy, under Contract No. DE-FG05-86ER53217 with Auburn University.

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