

Electron-impact ionization of multiply charged manganese ions

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(Received 11 May 2000; published 12 December 2000)

Distorted-wave calculations are carried out for the electron-impact ionization of atomic ions in the Mn isonuclear sequence. Detailed level to level calculations are performed for the dominant excitation-autoionization contributions. The validity of the configuration-average approach is studied and used to calculate direct ionization and higher n excitation-autoionization, when the level to level approach proves computationally too demanding. A combination of the two methods is used to analyze the recent crossed-beams experimental measurements of Mn^{5+} , Mn^{6+} , Mn^{7+} , and Mn^{8+} by Rejoub and Phaneuf [Phys. Rev. A **61**, 032706 (2000)]. The comparison between theory and experiment indicates that a large fraction of the initial population of each measured ion is in metastable states of excited configurations.

DOI: 10.1103/PhysRevA.63.012712

PACS number(s): 34.80.Kw

I. INTRODUCTION

A detailed understanding of electron collision dynamics involving multiply charged atomic ions remains a key factor in modeling the behavior of many astrophysical and laboratory plasmas [1,2]. An experimental and theoretical challenge is the determination of accurate electron-impact single ionization cross sections for the transition metal ions. Extensive work has been done for atomic ions in the Fe and Ni isonuclear sequences, as summarized in [3,4]. A recent experimental effort has revisited the low-charged ions in the Ti and Fe isonuclear sequences [5,6], with a few of the ions measured at very high energy resolution. Quite recently, absolute single ionization cross sections for several Mn ions have been measured using a new dynamic crossed-beams apparatus [7], prompting the theoretical investigations reported below.

The theoretical challenge in the determination of accurate electron ionization cross sections for transition metal ions is multifold. Direct ionization from the outer subshells results in the emission of two electrons in the long-range Coulomb field of the residual ion, the quantum three-body problem. Recent nonperturbative close-coupling studies along the Na isoelectronic sequence [8] have shown that first-order distorted-wave theory should yield accurate direct ionization cross sections for multiply charged ions (target charge of 3+ or greater). Indirect ionization from excitation of inner subshells followed by autoionization should again be accurately treated by first-order distorted-wave theory for multiply charged ions. Complications arise in both direct and indirect ionization from the sheer number of ground and excited levels found in the open shell transition metal ions. Thus, it is important to be able to apply level averaging methods, where possible, to obtain accurate total ionization cross sections.

The rest of this paper is organized as follows. In Sec. II, we give a brief review of the distorted-wave theory applied to electron-impact ionization, and in Sec. III we present electron-impact ionization cross sections for Mn^{5+} through Mn^{8+} calculated using level to level and configuration-average distorted-wave methods. We conclude with a brief summary in Sec. IV.

II. THEORY

The electron-impact ionization of an atomic ion is generally dominated by two processes; direct ionization:

$$e^- + A^{q+} \rightarrow e^- + A^{(q+1)+} + e^- \quad (1)$$

and excitation-autoionization:

$$e^- + A^{q+} \rightarrow (A^{q+})^* + e^- \rightarrow e^- + A^{(q+1)+} + e^-, \quad (2)$$

where A is an arbitrary ion with charge q and the $*$ signifies an autoionizing state. The total ionization is given by

$$\sigma_T(g \rightarrow f) = \sigma_{DI}(g \rightarrow f) + \sigma_{EA}(g \rightarrow f), \quad (3)$$

where $\sigma_{DI}(g \rightarrow f)$ is the direct ionization cross section and $\sigma_{EA}(g \rightarrow f)$ is the excitation-autoionization cross section from an initial level g to a final level f . The excitation-autoionization cross section through innershell excitation to an intermediate autoionizing level j is given by

$$\sigma_{EA}(g \rightarrow f) = \sum_j \sigma_E(g \rightarrow j) B_a(j \rightarrow f), \quad (4)$$

where $\sigma_E(g \rightarrow j)$ is the excitation cross section from level g to level j and $B_a(j \rightarrow f)$ is the multiple branching ratio for autoionization from level j to level f , defined as

$$B_a(j \rightarrow f) = \left[\frac{A_a(j \rightarrow f) + \sum_i A_r(j \rightarrow i) B_a(i \rightarrow f)}{\sum_k A_a(j \rightarrow k) + \sum_i A_r(j \rightarrow i)} \right]. \quad (5)$$

Here, $A_a(j \rightarrow k)$ is the autoionizing rate from level j to level k and $A_r(j \rightarrow i)$ is the radiative rate from level j to any lower energy level i . This includes further autoionization from level i to level f allowing all possible secondary autoionization in the level to level calculations.

We neglect the resonant excitation followed by sequential double autoionization process (commonly known as REDA). To date there have been no REDA calculations for ions as complex as low-charged members of the transition metals.

Theoretical and experimental work [9–12] on Na-like Fe has shown that the REDA contribution is no more than 25% of the average total ionization cross section and is confined to a small energy range below the excitation-autoionization thresholds.

Level to level excitation-autoionization calculations are carried out using the relativistic distorted-wave method found in the HULLAC package [13]. In the level to level distorted-wave method, the atomic structure is calculated using the fully relativistic multiconfigurational RELAC code [14], based on the parametric potential model [15]. The central potential is introduced as an analytic function of screening parameters that are determined by minimizing the first-order relativistic energy of a set of configurations. The excitation cross sections are then calculated in the distorted-wave approximation. This package uses the factorization-interpolation method [16], which significantly improves the efficiency of the radial integral calculations. Using this approach, we can solve Eq. (4) including many thousands of levels in our excitation model.

The configuration-average distorted-wave approximation [17] is used to calculate all of the direct ionization and some of the excitation-autoionization processes described in this paper. The threshold energies and the bound radial orbitals for the Mn configurations are calculated using the relativistically corrected Hartree-Fock atomic structure code of Cowan [18,19], where we include the mass-velocity and Darwin terms in the radial Schrödinger equation. The continuum radial orbitals are calculated as distorted-wave solutions of the relativistic radial Schrödinger equation using configuration-average Hartree and semiclassical exchange potentials [20]. The first-order scattering amplitude for either the ionization or excitation process is then averaged over all states of an initial configuration and summed over all states of a final configuration. The excitation amplitude is evaluated using incident and scattered electrons calculated in a V^N potential, where N is the number of target electrons. The ionization amplitude is also evaluated using incident and scattered electrons calculated in a V^N potential while the bound and ejected electrons are calculated in a V^{N-1} potential [21,22].

III. RESULTS

A. Comparison of detailed level to level and configuration-average distorted-wave calculations for Mn^{6+} innershell excitation

Total excitation cross sections from the ground configuration of Mn^{6+} ($3s^23p^63d$) to the $3s^23p^53dnl$ ($n=4,5,6$) and $3s3p^63dnl$ ($n=3,4,5$) excited configurations are presented in Fig. 1. The solid line is the cross section calculated using the level to level relativistic distorted-wave code for excitation from the $3s^23p^63d^2D_{3/2}$ level to all levels of the excited configurations. We note that excitation from the $3s^23p^63d^2D_{5/2}$ level is almost identical to excitation from the $^2D_{3/2}$. The dashed line is the total configuration-average cross section for the transitions above. The very good agreement between these curves is a good check on the configuration-average approach.

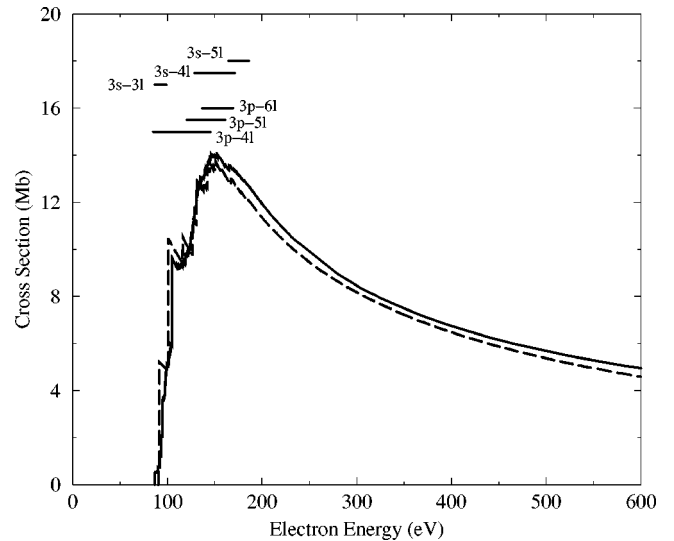


FIG. 1. Electron-impact excitation cross section from the ground configuration of Mn^{6+} to the $3s^23p^53dnl$ ($n=4,5,6$) and $3s3p^63dnl$ ($n=3,4,5$) excited configurations. The solid line is a calculation using the relativistic level to level distorted-wave program for excitation from the $3s^23p^63d^2D_{3/2}$ level. This is almost identical to the excitation from the $3s^23p^63d^2D_{5/2}$ level (not shown). The dashed line is using the configuration-average distorted-wave method.

The configuration-average method calculates the cross section from all levels of the initial configuration to all levels of each final configuration. In some cases this can cause difficulties. The final excited configuration can have levels spanning the ionization threshold, so when calculating excitation-autoionization cross sections one must be careful to include only the excitation to levels that, energetically, will contribute to excitation-autoionization. For this reason we have used, in subsequent calculations, the relativistic level to level distorted-wave program to calculate the excitation-autoionization for levels near the ionization threshold. For higher n levels the configuration-average approach is appropriate, since the levels are all well above the ionization threshold and so will all contribute to excitation-autoionization. Also, the detailed relativistic distorted-wave method proves computationally too demanding for these many high-lying levels.

Calculations from excited configurations can also cause problems. In some cases all of the levels in an excited configuration may not be populated, as they can quickly radiate down to the ground configuration; that is, not all of the levels within an excited configuration are metastable. Since the configuration-average approach averages over all initial levels, this may lead to inaccuracies. A level to level distorted-wave calculation is therefore more appropriate in situations where some of the excited levels are not fully populated. The relativistic level to level distorted-wave calculations include the branching ratio between autoionization and radiative decay in the excitation-autoionization calculations, also including the secondary autoionization processes discussed in the previous section. For high n levels, the relative contribution to the total ionization cross section is small so we can make

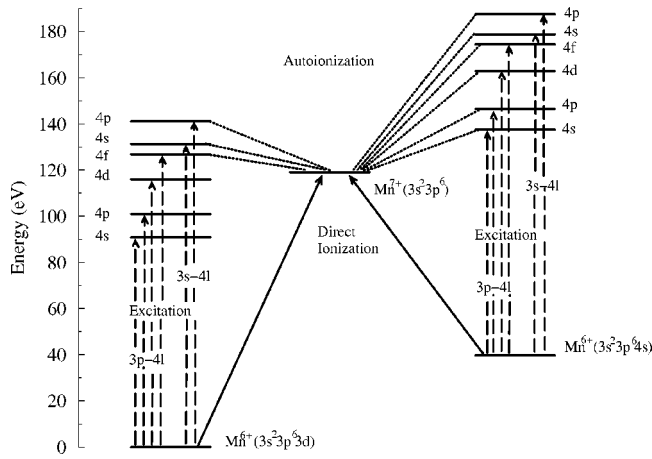


FIG. 2. Energy-level diagram for ionization of Mn^{6+} . The direct ionization and some excitation-autoionization routes from the ground and excited configurations are indicated.

a further approximation by assuming that the branching ratio for these excitations is close to one.

Therefore, a judicious use of the configuration-average approach, coupled with the level to level relativistic distorted-wave method when appropriate, enables accurate calculations of electron-impact ionization cross sections for the multiply charged Mn ions. This methodology has been used for the remaining calculations presented in this paper.

B. Ionization of Mn^{6+}

An energy-level diagram showing the direct ionization and some excitation-autoionization pathways ($3l-4l'$) for the ionization of Mn^{6+} (which is K-like) is shown in Fig. 2. Only some of the many excitation pathways are shown for clarity. We see that, from the ground configuration, only excitation from the $3p-4f$ and $3s-4l$ configurations leads to autoionization, whereas from the excited configuration all excitations shown lead to autoionization. We expect then that the ionization rate from the excited configuration will be greater than that from the ground configuration simply due to the greater number of pathways for excitation-autoionization.

We use a combination of level to level and configuration-average distorted-wave approximations to calculate the ionization of Mn^{6+} , which is compared to experiment [7] in Fig. 3. Figure 3(a) shows the total ionization cross section of Mn^{6+} from the ground configuration ($3s^23p^63d$), which has an average ionization energy of 119 eV, and Fig. 3(b) shows the total ionization cross section from the first excited configuration ($3s^23p^64s$), which has an average ionization energy of 79 eV. In these and in subsequent figures, the dashed line shows the contribution of direct ionization to the total cross section, which is given by the solid line. In order to present only one curve, the total cross section contains the combination of the metastable-average level to level calculation with the configuration-average calculation for the higher n configurations, where the metastable-average contribution is given by the average of only those levels within an configuration that are metastable. For Mn^{6+} , direct ionization from the $3d$, $3p$, and $3s$ subshells and $4s$, $3p$, and $3s$ sub-

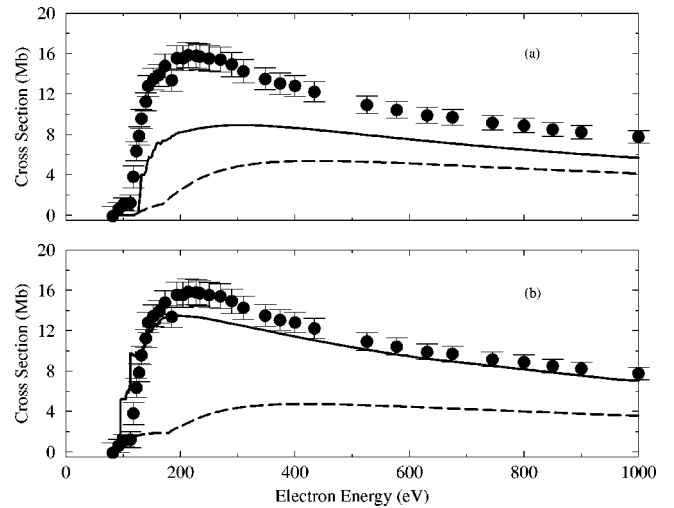


FIG. 3. Electron-impact total cross section for the ionization of Mn^{6+} from the (a) ground ($3s^23p^63d$) and (b) excited ($3s^23p^64s$) configurations. The experimental points are from Rejoub and Phaneuf [7]. The dashed line is the direct ionization contribution and the solid line is the total cross section. The total ionization from the ground configuration includes excitation-autoionization from $3s^23p^63d-3s^23p^53dnl$ ($n=4,5,6$) and $3s^23p^63d-3s3p^63dnl$ ($n=4,5$) calculated using the relativistic level to level distorted-wave programs, averaged over the metastable levels. From the first excited configuration, the total ionization includes excitation-autoionization from $3s^23p^64s-3s^23p^54snl$ ($n=4,5,6$) and $3s^23p^64s-3s3p^64snl$ ($n=4,5$) using the same method. Additional excitation-autoionization of the $3p-nl$ ($n=7,8,9$) and $3s-nl$ ($n=6,7,8$) calculated using the configuration-average distorted-wave approach is also included for both configurations.

shells, from the ground and excited configurations respectively, is included in a configuration-average calculation. The direct ionization cross section shown here is in good agreement with a semiempirical calculation based on the Lotz formula for estimating cross sections [23] (not reproduced here for clarity). From the ground configuration, excitation-autoionization from $3s^23p^63d-3s^23p^53dnl$ ($n=4,5,6$) and $3s^23p^63d-3s3p^63dnl$ ($n=4,5$) is calculated using the level to level relativistic distorted-wave programs described previously, and from the first excited configuration, excitation-autoionization from $3s^23p^64s-3s^23p^54snl$ ($n=4,5,6$) and $3s^23p^64s-3s3p^64snl$ ($n=4,5$) is calculated by the same method. Excitation-autoionization due to $\Delta n=0$ transitions (i.e., to the $3d$ shell) is not energetically possible. Additional excitation-autoionization of the $3p-nl$ ($n=7,8,9$) and $3s-nl$ ($n=6,7,8$) is calculated using the configuration-average distorted-wave method.

For the ground configuration of Mn^{6+} there are two levels, $3s^23p^63d^2D_{1/2,3/2}$, and for the first excited configuration there is only one level, $3s^23p^64s^2S_{1/2}$. The $3s^23p^64s^2S_{1/2}$ is the one and only metastable level and so we expect the configuration-average approach to work well for Mn^{6+} , since we will not encounter any problems associated with many levels in an excited configuration. The detailed level to level relativistic distorted-wave excitation-autoionization calculations for the innershell transitions defined above in-

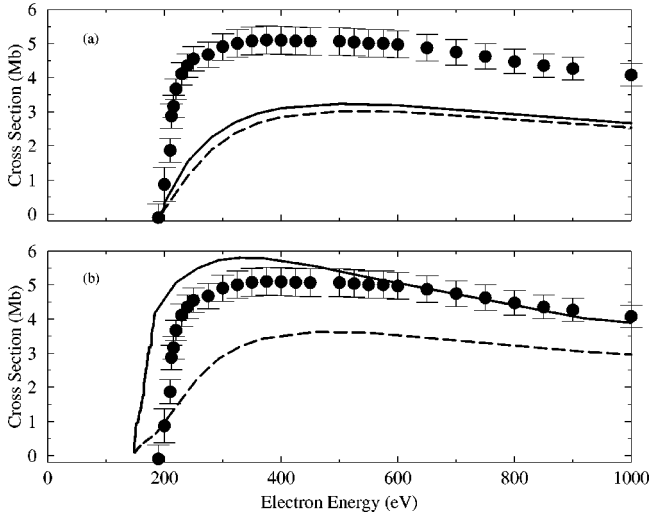


FIG. 4. Electron-impact total cross section for the ionization of Mn^{7+} from the ground ($3s^23p^6$) and first excited ($3s^23p^53d$) configurations. The lines are the same as in the previous figure. The total ionization from the ground configuration (a) includes excitation-autoionization from $3s^23p^6-3s3p^65l$ calculated using the relativistic level to level distorted-wave programs averaged over the metastable levels and $3s^23p^6-3s3p^6nl$ ($n=6,7,8$) calculated using the configuration-average distorted-wave programs. In the first excited configuration (b) excitation-autoionization of the $3p-nl$ ($n=4,5$), calculated using the level to level distorted-wave programs, and $3p-nl$ ($n=6,7,8,9$) and $3s-nl$ ($n=4-9$) calculated using the configuration-average programs, are all included in the total cross section.

clude all possible radiative transitions and multistep autoionizations that involve 1990 levels. For high n levels, we have assumed that the branching ratio for autoionization is still close to one. This will not be strictly true for high n levels, but since the excitation-autoionization cross section from these levels is relatively small in any case, this is unlikely to introduce a large error into our calculation.

The total cross section calculated from the ground state of Mn^{6+} is significantly lower than the experimental measurements [7], and although at higher energies the cross section from the excited configuration falls within the experimental error bars, it fails to reproduce the peak at around 230 eV. It should also be noted that a calculation has been performed where all excitation-autoionization is calculated using the configuration-average method only, and it is found that this yields a similar result to Fig. 3.

C. Ionization of Mn^{7+}

We use a combination of level to level and configuration-average distorted-wave approximations to calculate the ionization of Mn^{7+} and compare to experiment [7] in Fig. 4. Figure 4(a) shows the ionization cross section from the ground configuration ($3s^23p^6$) that has an average ionization threshold of 195 eV, and Fig. 4(b) shows the ionization cross section from the excited configuration ($3s^23p^53d$) that has an average ionization threshold of 145 eV. Mn^{7+} is a member of the Ar-like isoelectronic sequence and so the ground configuration has a closed outer shell. Direct ioniza-

tion from the $3p$ and $3s$ subshells is included in the configuration-average calculation for the ground configuration, and from the $3d$, $3p$, and $3s$ subshells in the calculation for the excited configuration.

As expected, the direct ionization dominates the ionization from the ground configuration, which has only one level $3p^6\ ^1S_0$, since the closed-shell nature limits the contribution of excitation-autoionization. The direct ionization is in good agreement with a semiempirical Lotz calculation. The small excitation-autoionization contributions to the cross section from the $3s^23p^6-3s3p^65l$ transition (calculated using the level to level relativistic distorted-wave code) and from the $3s^23p^6-3s3p^6nl$ ($n=6,7,8$) transitions (calculated using the configuration-average distorted-wave approach) give the total ionization cross section. There is no contribution from excitation of the $3p$ subshell. Again, the $3s-5l$ excitation-autoionization is calculated using the level to level distorted-wave code since not all of the levels associated with the $5l$ configuration lead to autoionization.

The first excited configuration ($3s^23p^53d$) of Mn^{7+} contains 12 levels, of which three, with $J=1$, are not metastable, since the only radiatively allowed transition is from $J=1$ to $J=0$. Excitation-autoionization is calculated using the detailed level to level distorted-wave method involving the inner-shell transitions $3s^23p^53d-3s^23p^43dnl$ ($n=4,5$) in which we include in our model all possible radiative transitions that involve 1998 levels in total. The $3p-4d$ and $3p-4f$ excitations are selective processes dominated by only a few transitions and so it is important to identify the position of each final level relative to the ionization limit.

Among the excited configuration levels, the $3p^53d\ ^1P_1$ level has a substantially larger total excitation cross section than the other excited levels and also an ionization threshold that is 20 eV below that of the other levels. This is a common feature of 1P_1 levels arising from open p and d shells, as in this configuration. This level, which is not metastable, is inevitably included in the configuration-average distorted-wave calculation and the large (around 25%) difference in the total excitation cross section could introduce inaccuracies in our final results. However, the statistical weight of this level (1P_1) is relatively low and it is found that the difference between the metastable-averaged and configuration-averaged excitation cross section, for the $3s^23p^53d-3s^23p^43dnl$ ($n=4,5$) transition is only 6%.

The $3s^23p^53d-3s^23p^43dnl$ ($n=6,7,8,9$) and $3s^23p^53d-3s3p^53dnl$ ($n=4,5,6,7,8,9$) excitation-autoionization cross sections are calculated using the configuration-average distorted-wave method. The higher n excitations are all well above the ionization threshold so that the difference in the threshold energies from the 1P_1 and the rest of the levels in the excited configuration becomes relatively smaller. The total excitation-autoionization contribution from the first excited configuration is much larger, as would be expected from the much lower ionization threshold, since more autoionizing channels are now open.

The total ionization from the ground configuration is much smaller than the experimental results. The total ionization from the excited configuration is larger than the experimental points at low energy, although there is good agree-

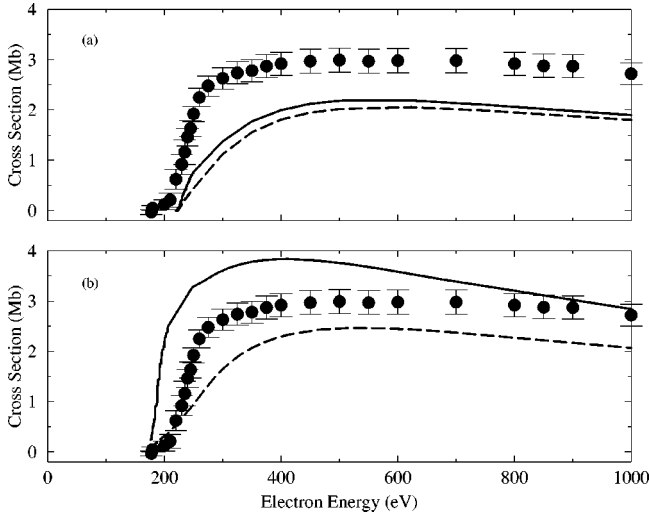


FIG. 5. Electron-impact total cross section for the ionization of Mn^{8+} from the ground ($3s^23p^5$) and first excited ($3s^23p^43d$) configurations. The lines are the same as in the previous figure. The total ionization from the ground configuration (a) includes excitation-autoionization from $3s^23p^5-3s3p^55l$ calculated using the relativistic level to level distorted-wave programs averaged over the metastable levels, and $3s^23p^5-3s3p^5nl$ ($n=6,7,8,9$) using the configuration-average distorted-wave approach. In the ionization from the first excited configuration (b) excitation-autoionization of the $3p-nl$ ($n=4,5$), calculated using the level to level distorted-wave programs, and $3p-nl$ ($n=6,7,8,9$) and $3s-nl$ ($n=4-9$) calculated using the configuration-average programs, are all included in the total cross section, as previously.

ment at higher energies. The large discrepancy between the experimental results and the ionization from the ground configuration seems to indicate that the excited component is present in the ion beam in this experiment. Unfortunately, there are not enough experimental points at low energy to determine if ionization below the ground-state threshold is observed; that is, an ionization contribution in the energy range just above the excited-configuration threshold.

D. Ionization of Mn^{8+}

Calculations of the total ionization cross section of Mn^{8+} are presented in Figs. 5(a) and 5(b), from the ground ($3s^23p^5$) and excited ($3s^23p^43d$) configurations, respectively, and again compared to experimental results [7]. Mn^{8+} is Cl-like, with a ground-state average ionization threshold of 223 eV. The average ionization threshold of the excited configuration is 172 eV. Direct ionization from the $3p$ and $3s$ shells (and from the $3d$ shell for the excited configuration) are calculated using the configuration-average distorted-wave method. Again the direct ionization calculations agree well with a semiempirical calculation based on the Lotz formula.

The ground configuration of Mn^{8+} has only two levels, $3p^5\ ^2P_{1/2,3/2}$ of which the $\ ^2P_{3/2}$ is slightly lower. Excitation-autoionization of $3s^23p^5-3s3p^55l$ is calculated using the level to level relativistic distorted-wave code since not all of the levels associated with the $3s3p^55l$ configuration are above the ionization threshold. Excitation-autoionization of

$3s^23p^5-3s3p^5nl$ ($n=6,7,8,9$) is calculated using the configuration-average distorted-wave method since these levels are all well above the ionization threshold. There is no contribution to excitation-autoionization from excitation of the $3p$ subshell. As expected, the direct ionization again dominates the cross section and as previously the total ionization cross section is much lower than the experimental results [7].

The first excited configuration ($3s^23p^43d$) of Mn^{8+} contains 28 levels, of which only 7 (having $J=7/2$ or $9/2$) are metastable. Excitation-autoionization is calculated using the detailed level to level distorted-wave method involving the innershell $3s^23p^43d-3s^23p^33dnl$ ($n=4,5$) transitions in which all possible radiative transitions are included. This very large calculation (which for the ground and excited configurations involves 2842 levels) is necessary to obtain the correct cross section for these transitions as only some of the levels of the excited configuration are metastable. We compared the metastable-averaged excitation cross section to the configuration-averaged cross section for the $3s^23p^43d-3s^23p^33dnl$ ($n=4,5$) transition and found a difference of 15%. The $3s^23p^43d-3s^23p^33dnl$ ($n=6,7,8,9$) and $3s^23p^43d-3s3p^43dnl$ ($n=4,5,6,7,8,9$) excitation-autoionization cross sections are calculated from the configuration-average distorted-wave method. Although we would expect some difference in the configuration-average results for these higher n transitions compared to a full level to level calculation, the absolute error will be much less since these excitation-autoionization cross sections are smaller.

It is clear in Mn^{8+} that the experimental results [7] contain a large proportion of ions in the metastable levels due to the significant ionization contribution below the ground-state threshold. A combination of the theoretical results in Figs. 5(a) and 5(b) must be considered in any comparison with the experimental measurements. A determination of the fraction of ions in the excited configuration present in the experiment will enable a better understanding of these results.

E. Ionization of Mn^{5+}

To complete the comparison with recent experimental results [7], the total ionization cross sections for Mn^{5+} ionization, from the ground ($3s^23p^63d^2$) and first excited ($3s^23p^63d4s$) configurations are presented in Figs. 6(a) and 6(b), respectively. Mn^{5+} is Ca-like, with an average ionization potential from the ground configuration of 94 eV and of 64 eV from the excited configuration. These calculations were carried out using only the configuration-average distorted-wave method, as relativistic level to level distorted-wave calculations for these levels prove computationally very demanding due to the large number of levels present in the configurations. However, in light of our previous results (discussed above), we expect that these calculations are reasonably close to full level to level calculations.

The direct ionization (dashed line) includes ionization from the $3d$, $3p$, and $3s$ shells (from the ground configuration) and $4s$, $3d$, $3p$, and $3s$ shells (from the excited configuration). All excitation-

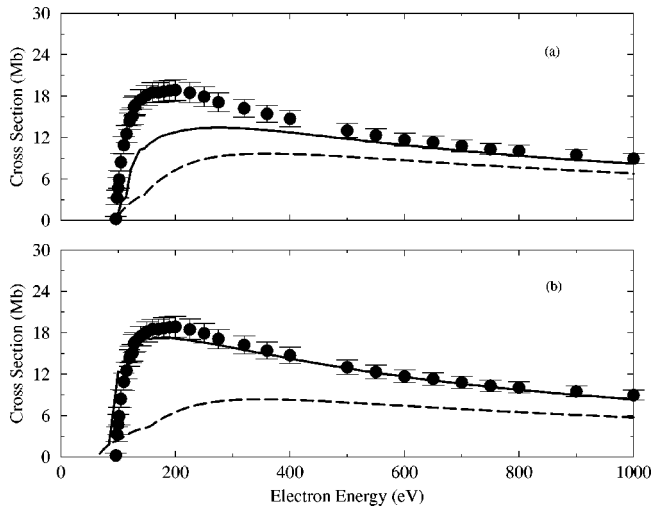


FIG. 6. Electron-impact total cross section for the ionization of Mn^{5+} from the (a) ground ($3s^2 3p^6 3d^2$) and (b) first excited ($3s^2 3p^6 3d 4s$) configurations. The lines are the same as in the previous figure. Excitation-autoionization from $3s^2 3p^6 3d^2 - 3s^2 3p^5 3d^2 nl$ ($n=4-8$) and $3s^2 3p^6 3d^2 - 3s 3p^6 3d^2 nl$ ($n=4-7$), calculated solely using the configuration-average distorted-wave method, is included in the cross-section calculation from the ground configuration. From the excited configuration, all excitation-autoionization from $3s^2 3p^6 3d 4s - 3s^2 3p^5 3d 4s nl$ ($n=4-8$) and $3s^2 3p^6 3d 4s - 3s 3p^6 3d 4s nl$ ($n=4-7$) is included in the configuration-average distorted-wave calculation.

autoionization from $3s^2 3p^6 3d^2 - 3s^2 3p^5 3d^2 nl$ ($n=4-8$) and $3s^2 3p^6 3d^2 - 3s 3p^6 3d^2 nl$ ($n=4-7$) is included in the calculation from the ground configuration, and excitation-autoionization from $3s^2 3p^6 3d 4s - 3s^2 3p^5 3d 4s nl$ ($n=4-8$) and $3s^2 3p^6 3d 4s - 3s 3p^6 3d 4s nl$ ($n=4-7$) is included in the calculation from the excited configuration. The cross section from the excited configuration is larger than that from the

ground configuration as in the previous ions studied; it is again postulated that the experimental results [7] contain a combination of ionization from both the ground configuration and metastable levels in the excited configuration.

IV. SUMMARY

In this paper, we have investigated the electron-impact ionization of Mn^{q+} ($q=5-8$) in comparison with a recent crossed-beams experiment [7]. We have calculated the direct ionization using a configuration-average method and demonstrated the validity of this approach for excitation cross sections by comparisons with those obtained from large detailed calculations using an accurate level to level relativistic distorted-wave approach [13]. We find that a combination of these two methods is best suited, when possible, to calculating the total cross section for electron-impact ionization.

The agreement between our theoretical results from the ground configuration and experiment is generally poor, indicating a substantial population in metastable states of the excited configuration. However, the failure of theory to, in most cases, reproduce the shape of the experimental plots gives cause for concern. In our calculations we have not included the possibility of ionization from the L shell (i.e., ionization of $2p$ electrons), because of the large probability for double ionization at these higher energies. This may contribute to the slow falloff of some of the experimental curves, but as this is only energetically allowed at high energies, it will not explain the disagreements near the peak of the ionization. It is hoped that further experiments, where the ions are all in well-known atomic configurations, can shed some light on these discrepancies.

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Department of Energy. Computational work was carried out at the National Energy Research Supercomputer Center at Lawrence Berkeley National Laboratory.

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- [1] *Atomic and Molecular Processes in Fusion Edge Plasmas*, edited by R. K. Janev (Plenum, New York, 1995).
 - [2] *Stellar Evolution, Stellar Explosions, and Galactic Chemical Evolution*, edited by A. Mezzacappa (Institute of Physics, London, 1998).
 - [3] M.S. Pindzola, D.C. Griffin, C. Bottcher, S.M. Younger, and H.T. Hunter, *Nucl. Fusion Suppl.* **1**, 21 (1987).
 - [4] M.S. Pindzola, D.C. Griffin, C. Bottcher, M.J. Buie, and D.C. Gregory, *Phys. Scr.*, T **37**, 35 (1991).
 - [5] U. Hartenfeller, K. Aichele, D. Hathiramani, G. Hofmann, V. Schafer, M. Steidl, M. Stenke, E. Salzborn, and M.S. Pindzola, *J. Phys. B* **31**, 2999 (1998).
 - [6] M. Stenke, K. Aichele, U. Hartenfeller, D. Hathiramani, M. Steidl, and E. Salzborn, *J. Phys. B* **32**, 3627 (1999).
 - [7] R. Rejoub and R.A. Phaneuf, *Phys. Rev. A* **61**, 032706 (2000).
 - [8] N.R. Badnell, M.S. Pindzola, I. Bray, and D.C. Griffin, *J. Phys. B* **31**, 911 (1998).
 - [9] K.J. LaGattuta and Y. Hahn, *Phys. Rev. A* **24**, 2273 (1981).
 - [10] S.S. Tayal and R.J.W. Henry, *Phys. Rev. A* **39**, 3890 (1989).
 - [11] M.H. Chen, K.J. Reed, and D.L. Moores, *Phys. Rev. Lett.* **64**, 1350 (1990).
 - [12] J. Linkemann, A. Müller, J. Kenntner, D. Habs, D. Schwalm, A. Wolf, N.R. Badnell, and M.S. Pindzola, *Phys. Rev. Lett.* **74**, 4173 (1995).
 - [13] J. Oreg, W.H. Goldstein, M. Klapisch, and A. Bar-Shalom, *Phys. Rev. A* **44**, 1750 (1991).
 - [14] M. Klapisch, J.L. Schwob, B.S. Frankel, and J. Oreg, *J. Opt. Soc. Am.* **67**, 148 (1977).
 - [15] M. Klapisch, *Comput. Phys. Commun.* **2**, 239 (1971).
 - [16] A. Bar-Shalom, M. Klapisch, and J. Oreg, *Phys. Rev. A* **38**, 1773 (1988).
 - [17] M.S. Pindzola, D.C. Griffin, and C. Bottcher, in *Atomic Processes in Electron-Ion and Ion-Ion Collisions*, Vol. 145 of *NATO Advance Studies Institute, Series B: Physics*, edited by

- F. Brouillard (Plenum, New York, 1986), p. 75.
- [18] R.D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
- [19] R.D. Cowan and D.C. Griffin, *J. Opt. Soc. Am.* **66**, 1010 (1976).
- [20] M.E. Riley and D.G. Truhlar, *J. Chem. Phys.* **63**, 2182 (1975).
- [21] S.M. Younger, *Phys. Rev. A* **22**, 111 (1980).
- [22] H. Jakobowicz and D.L. Moores, *J. Phys. B* **14**, 3733 (1981).
- [23] W. Lotz, *Z. Phys.* **216**, 241 (1968); **220**, 466 (1969).