Electron-impact ionization cross sections for the xenon isoelectronic sequence

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Cross sections are presented for the direct electron-impact ionization of the $5p$, $5s$, and $4d$ subshells of the ground state of the first six members of the xenon isoelectronic sequence. The calculations were performed in a distorted-wave Born-exchange approximation including the effects of term-dependent partial waves in the ejected-electron channel and ground-state electron correlation. Shape resonances were found to significantly enhance the cross sections at low incident electron energies for Xe, Cs^+, and Ba^{2+}. Term dependence in the $5p^5kd$ and $4d^9kf$ ejected-electron channels was also significant for these ions. Ground-state correlation was somewhat less influential, and affected the cross section only when ejected-electron term dependence was also significant.

I. INTRODUCTION

Heavy atoms and ions offer the atomic physicist an interesting opportunity to study the structure and dynamics of many-electron systems in a regime where many-body effects can have a profound influence on observables. This is especially true for $Z \geq 46$ where the $4d$ subshell is just filled. The large number of electrons occupying the N shell has been shown to lead to multiwell potentials for the higher-angular-momentum bound and scattering states, especially the f ($l=3$) channel which can strongly interact with the N shell.[1,2] For few-times-ionized atoms shape resonances associated with these multiwell potentials can qualitatively change the scattering cross sections involving high-angular-momentum partial waves.[3] Even for moderately ionized atoms up to $10\times$ionized there can be significant term-dependent potential effects.[4,5] Although some of these effects also occur for light atoms and ions, they are often much more pronounced at high Z.

In addition to the basic atomic-physics attraction of studying electron scattering from heavy atoms and ions, there are important practical applications of such data. The ionization balance and energy-transport properties of heavy ions in low-temperature plasmas are strongly influenced by electron-impact ionization. Very little experimental or theoretical information is available for atoms with $Z > 26$, so that estimates for heavy-ion electron ionization cross sections are often based on uncertain extrapolations from neutral atoms or simple semiclassical or semiempirical approximations. Recent studies[6] have shown that such simple methods can lead to gross errors in the prediction of plasma properties. Thus there is a need for further experiments and calculations addressing the unique features of heavy ions.

In this paper we report the results of calculations of electron-impact ionization cross sections for the first six ions of the xenon isoelectronic sequence. The calculations were performed using a distorted-wave Born-exchange approximation including the effects of partial-wave angular term dependence and ground-state electron correlation. The xenon sequence offers several advantages for studying the properties of heavy atoms and ions. It has a closed-shell ground state leading to a simple description of the scattering waves at least at the distorted-wave level of approximation. Target correlation is a significant influence on the cross section, yet is compactly represented by a single optimized pair excitation from the subshell under consideration. The ejected channels of both valence and inner-core subshells can be highly dependent on the term value of the channel, offering insights into the ejected-electron–residual-ion interaction. Contributions to the cross section due to excitation-autoionization types of resonances should be small for xenonlike ions, allowing a relatively clean comparison of the theoretical prediction for the direct ionization cross section with experimental data. The appearance of shape resonances in the cross sections for $4d$-subshell ionization in Xe, Cs^+, and Ba^{2+} has already been discussed in a previous paper.[7] The present work extends these earlier calculations to higher charge states and also investigates the ionization of the $5s$ and $5p$ subshells.

Section II contains a brief description of the theoretical approximation employed. Section III presents the results of the calculations, concentrating on the variation of the shape and amplitude of the cross sections versus channel term dependence in the ejected channel and the occurrence of shape resonances in the scattered-wave channel. Section IV concludes the paper, and suggests opportunities for further theoretical and experimental study.

II. THEORETICAL METHOD

Details of the distorted-wave Born-exchange method employed here have been given elsewhere,[7–9] and only a brief description will be presented here. The electron-impact ionization cross section was approximated by a triple partial-wave expansion over the incident-, scattered-, and ejected-electron channels and an integration over the allowed energy distribution in the two-continuum-electron final state. Hartree-Fock wave functions were employed to describe the target.[10] Both the initial- and final-state bound configurations were constructed from initial ground-state orbitals. Unless otherwise noted, partial waves were computed in a semiclassical exchange (SCE) approximation[11] to the Hartree-Fock potential of the initial target configuration (incident and scattered waves) or the ionized configuration (ejected waves). The maximum-interference approximation of Peterkop[12] was used for the phase of the exchange matrix element. Note that there are two types of exchange in the cross-section calculation: scattering exchange, which involves the exchange between the two final-state continuum electrons, and potential exchange, which occurs between a specific continuum wave and the target electrons.

The $5p^5kd\ ^1P$ and the $4d^9kf\ ^1P$ channels which appear in the electron-ionization matrix element for the ^1S initial target state of xenonlike ions are known to be sensitive to the term value of the channel. In these cases nonlocal term-dependent Hartree-Fock (TDHF) calculations of the ejected partial waves were performed using the potentials[13]

$$\begin{aligned} V_{\rm TDHF}P_{kf} = V_{\rm CA}P_{kf} - [&\tfrac{24}{105}Y^2(4d,4d,r) \\ &+ \tfrac{66}{693}Y^4(4d,4d,r)]P_{kf} \\ &+ [\tfrac{137}{70}Y^1(4d,kf,r) - \tfrac{2}{105}Y^3(4d,kf,r) \\ &- \tfrac{55}{2541}Y^5(4d,kf,r)]P_{4d} \end{aligned} \quad (1)$$

for the $4d^9kf\ ^1P$ channel and

$$\begin{aligned} V_{\rm TDHF}P_{kd} = V_{\rm CA}P_{kd} &- \tfrac{1}{5}Y^2(5p,5p,r)P_{kd} \\ &+ [\tfrac{19}{15}Y^1(5p,kd,r) - \tfrac{3}{70}Y^3(5p,kd,r)]P_{5p} \end{aligned} \quad (2)$$

for the $5p^5kd\ ^1P$ channel. $V_{\rm CA}$ is the potential for the configuration average[14] of the respective configuration and

$$\begin{aligned} Y^k(nl,n'l',r) = (1/r^{k+1})\int P_{nl}(x)x^kP_{n'l'}(x)dx \\ + r^k\int P_{nl}(x)(1/x^{k+1})P_{n'l'}(x)dx \ . \end{aligned} \quad (3)$$

The large positive coefficient of the dipole exchange integral Y^1 repels the continuum wave from the subshell being ionized, causing significant changes in the cross section.

Ground-state electron correlation of the type $5p^6+5p^45d^2$ was included for the $5p$-subshell ionization calculations. For $4d$ ionization the analogous pair excitation $4d^{10}+4d^84f^2$ was included. These excitations are expected to represent the dominant corrections to the ground-state wave functions for the initial target.[15,16] Note that selection rules within the matrix element allow ground-state correlation to affect the scattering matrix element only so long as there is significant term dependence in the ejected-electron channel which causes nonorthogonality between the correlation orbital and the ejected wave of the same symmetry.[5] As Z increases, the term dependence of the ejected channel decreases and the orthogonality between the continuum wave and the correlation orbital improves. This implies that the effect of target-electron correlation on the cross section also decreases with increasing Z.

Ionization energies used in the present work are given in Table I. Measured values[17,18] were employed where they were available. Otherwise, a theoretical ionization energy was derived from the difference in the Hartree-Fock total energies of the initial and final target configurations.

TABLE I. Ionization energies of xenonlike ions (a.u.).

Ion	I_{5p}	I_{5s}	I_{4d}
Xe	0.4458[a]	0.8438[a]	2.584
Cs^+	0.9216[a]	1.483[a]	3.387
Ba^{2+}	1.303	1.908	4.263
La^{3+}	1.836[a]	2.454[a]	5.220
Ce^{4+}	2.409[a]	3.100[a]	6.264
Pr^{5+}	3.014	3.796	7.378

[a]Measured data, Refs. 17 and 18.

The distorted-wave method used here represents a first-order calculation of the interaction of the scattering electron with the many-electron target. For light atoms and ions it has been found to yield cross sections in excellent agreement with available experimental data, often to within 25%. Its suitability to describe electron scattering from heavy atoms is complicated by the complex structure of many-electron systems, as well as the many additional transition channels available for such targets. Nevertheless, the distorted-wave method is an intermediate step between a simple plane-wave Born approximation which omits any consideration of scattering-electron–target interaction and a full many-body calculation, the computational labor associated with which would be enormous.

III. CROSS SECTIONS

A. Ionization of the 5p and 5s subshells

Figure 1 compares the results of several calculations of the $5p$ and $5s$ cross sections computed in different theoretical approximations. The cross section Q, in units of πa_0^2 ($a_0=0.529\times10^{-8}$ cm), is plotted versus the energy of the incident electron u, measured in units of the ionization energy of the subshell. Four calculations are shown for the $5p$ cross section to illustrate the effects of adding scattering exchange, partial-wave term dependence, and ground-state correlation to the approximation for the scattering matrix element. The dotted curve is a simple distorted-wave calculation which neglects scattering exchange and which uses partial waves computed in a semiclassical exchange (SCE) approximation to the nonlocal Hartree-Fock exchange potential. The dashed curve is an SCE partial wave calculation including scattering exchange, i.e., a Born-exchange calculation. The dot-dashed curve is a Born-exchange cross section computed with term-dependent ejected d waves. The solid curve corresponds to a Born-exchange approximation including both term-dependent ejected waves and ground-state correlation of the type $5p^6+5p^45d^2$. Distorted-wave Born-exchange cross sections computed with SCE partial waves and a single-configuration target wave function are also shown for the $5s$ subshell. Experimental data for the single-ionization cross section are shown where they are available.

For Xe, Cs^+, and Ba^{2+} the $5p$ cross section is quite sensitive to the theoretical approximation employed. Whereas previous studies of electron ionization of few-electron ions indicated that scattering exchange exerts only a small effect on the cross section, in the low-ionization stages of the xenon sequence the effect is quite significant. Also, both the shape and amplitude of the cross section for these ions are strongly affected by term-dependent exchange terms in the potential describing the $5p^5kd\ ^1P$ channel. The explanation for this sensitivity can be found in the structure of the potentials determining the kd ejected waves, which dominate the cross section for low and intermediate incident electron energy. For few-times ionized Xe-like ions the potential governing high-l ejected partial waves consists of two negative wells separated by an intermediate potential barrier, which in some cases rises above zero energy. The inner well is formed from a combination of the central nuclear potential, the centrifugal term $l(l+l)/r^2$ in the kinetic energy operator, and the electrostatic electron-electron interaction. The barrier at intermediate radii is a result of the interelectronic interaction among the tightly localized M- and N-shell orbitals. The outer well represents the long-range screened nuclear potential, i.e., the asymptotic charge of the ion. If the direct part of the potential barrier separating the two wells is sufficiently large then ejected d waves will be roughly independent of the term value of the $5p^5kd$ configuration. The potential neglecting exchange will be sufficient to exclude low-energy partial waves from the radial region occupied by the core orbitals. Only high-energy partial waves will be able to penetrate the potential barrier and interact significantly with the tightly bound target orbitals.

Increasing the nuclear charge lowers the absolute value of the potential, although its shape remains roughly constant since the bound orbitals determining it do not undergo significant changes. The influence of the potential barrier on the partial waves is reduced, however, so it is no longer able to prevent the penetration of d waves into the atomic core. Only when the direct electrostatic potential is augmented by term-dependent exchange potentials can the effective amplitude of the barrier be increased to the point where it can significantly reduce d-

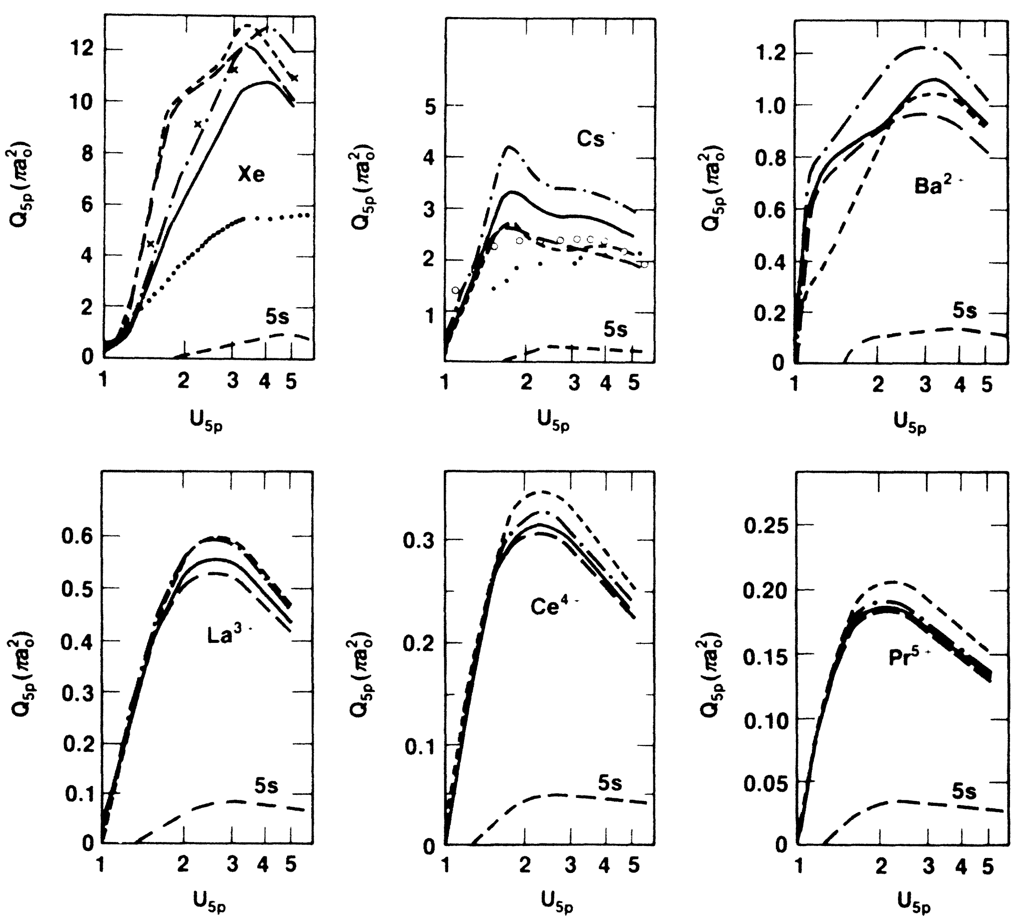

FIG. 1. Electron-impact ionization cross sections for ionization of the $5p$ and $5s$ subshells of the first six members of the xenon isoelectronic sequence. -----, distorted-wave calculation without scattering exchange using SCE partial waves; — — —, distorted-wave Born-exchange approximation using SCE partial waves; —·—·—·, distorted-wave Born-exchange approximation using term-dependent kd-ejected partial waves; ——, distorted-wave Born-exchange approximation using term-dependent kd-ejected partial waves and including ground-state electron correlation; ×, plane-wave Born approximation. Experimental data: Xe, ●, Wetzel *et al.* (Ref. 21); Cs^+, ○, Hertling *et al.* (Ref. 23); ●, Peart and Dolder (Ref. 22).

wave penetration into the core.

That the term-dependent cross section should increase rather than decrease for Cs^+ and Ba^{2+} when the partial waves are *repelled* from the core has been explained by Griffin *et al.*[19] They find that the cross section is strongly influenced by cancellation within the double integrand constituting the partial scattering matrix element, especially cancellation brought about by the overlap of the bound and ejected orbitals. As the ejected wave is repelled from the vicinity of the $5p$ subshell by the strong exchange interaction in the ^1P channel the cancellation within the matrix element decreases and the cross section increases. The term dependence of the $5p$ cross sections for La^{3+} and higher ions is much weaker than for Cs^+ and Ba^{2+}. This is because the potential barrier has become overwhelmed by the asymptotic Coulomb potential of the ion.

The effect of initial-state electron correlation of the type $5p^6+5p^45d^2$ is to reduce the cross section by roughly 0–20% for the different ions studied. The first-order description of electron scattering (the basis for the distorted-wave approximation) involves a single two-body Coulomb interaction. One of the channels is occupied by the scattering electron, the other by the electron being ionized. Target correlation consisting of pair correlations can affect the scattering matrix element only so long as the correlation orbitals in the target wavefunction are nonorthogonal to the ejected wave. Otherwise, there are not enough places in the transition operator to acommodate scattering, correlation excitations, and the ejection of a target electron.[5] The overlap term associated with orbitals not undergoing a Coulomb interaction will cause the matrix element to vanish. Thus target correlation is expected to be a significant effect on the cross section only when the ejected waves are nonorthogonal to the correlation orbitals, a situation which usually occurs only when there is strong term dependence in the ejected channel. As the nuclear charge increases along an isoelectronic sequence the orthogonality between the correlation orbital and the ejected wave improves, and the direct effect of electron correlation on the matrix element is reduced.

Ba^{2+} is an especially interesting ion from the perspective of scattering interactions, since a large enhancement is predicted in the cross section when scattering exchange is included. This qualitative change in the energy dependence of the cross section is due to the structure of the potentials which determine the partial waves appearing in the direct and exchange scattering matrix elements. In the direct matrix element the kf scattered wave, i.e., the more energetic of the two final-state electrons, is computed in the potential of the initial target. Its energy is sufficiently high to be independent of the effects of the potential barrier separating the inner and outer wells. The low-energy ejected orbital in the direct matrix element is computed in the potential of the Ba^{3+} ion, which is too highly ionized to exhibit pronounced resonant behavior. In the exchange matrix element the situation is reversed, however, and the slow electron is computed in the potential of the initial target, which contains a much more pronounced barrier.

Figure 2 illustrates the phase shifts for the kf scattered wave computed in the semiclassical exchange potential corresponding to the initial target ground state. For Xe

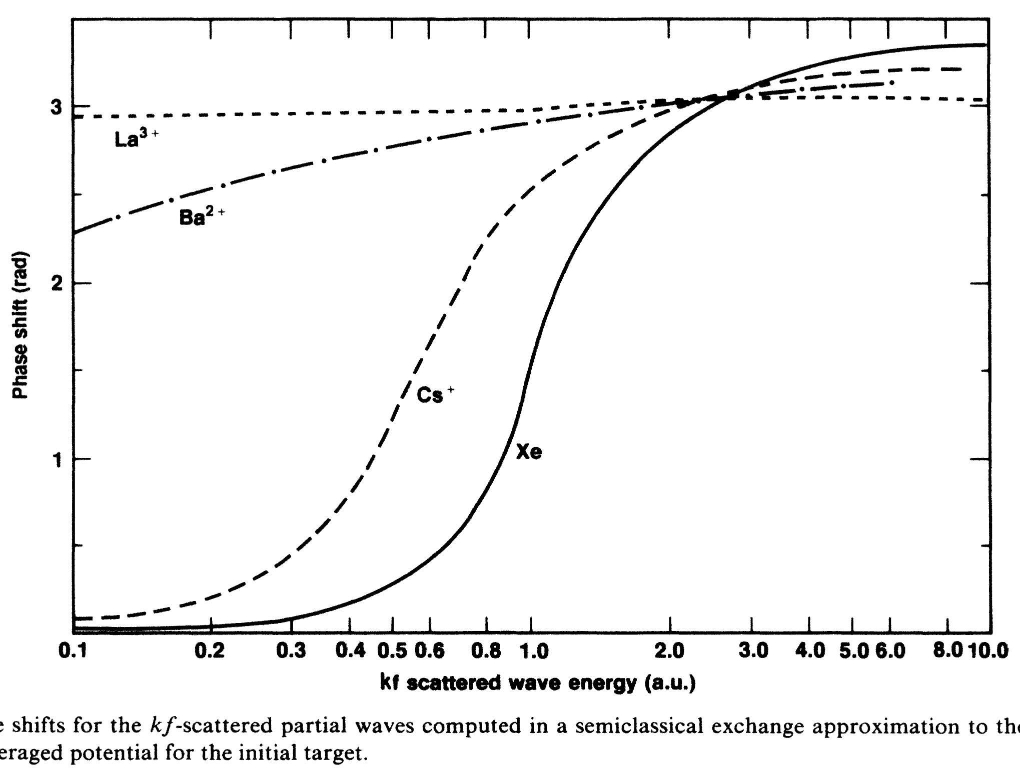

FIG. 2. Phase shifts for the kf-scattered partial waves computed in a semiclassical exchange approximation to the Hartree-Fock configuration-averaged potential for the initial target.

and Cs^+ the phase shift increases by π, indicating the presence of a shape resonance. As the nuclear charge is increased beyond $Z=55$ the scattering potential is no longer able to support a shape resonance. No other partial waves for the xenonlike ions examined were found to contain shape resonance.

Figure 3 compares the scaled cross sections I^2Q computed in the Born-exchange approximation including kd ejected-wave term dependence and ground-state correlation. Also shown is the prediction of the simple Lotz formula [20] $uI^2Q=2.77n\ \ln(u)$ which is often used in practical plasma-modeling calculations. Here Q is the cross section in units of πa_0^2, I is the ionization energy in rydbergs, and n is the number of electrons in the subshell being ionized. Comparison of the curves in Fig. 3 shows that the cross section for $5p$ ionization in Cs^+ peaks at very low incident electron energy compared to either Xe or more highly ionized ions. This anomalous shape in Cs^+ is the result of the kf scattered-wave channel passing through the shape resonance at approximately[3] 0.6 a.u. This resonance results in a very rapid rise in the Cs^+ electron-ionization cross section near threshold, as well as an unusual fall-off toward high incident electron energies. Since the resonance is in the scattered-electron channel, it can influence the ionization or excitation cross section of any Cs^+ bound orbital. Even though all three

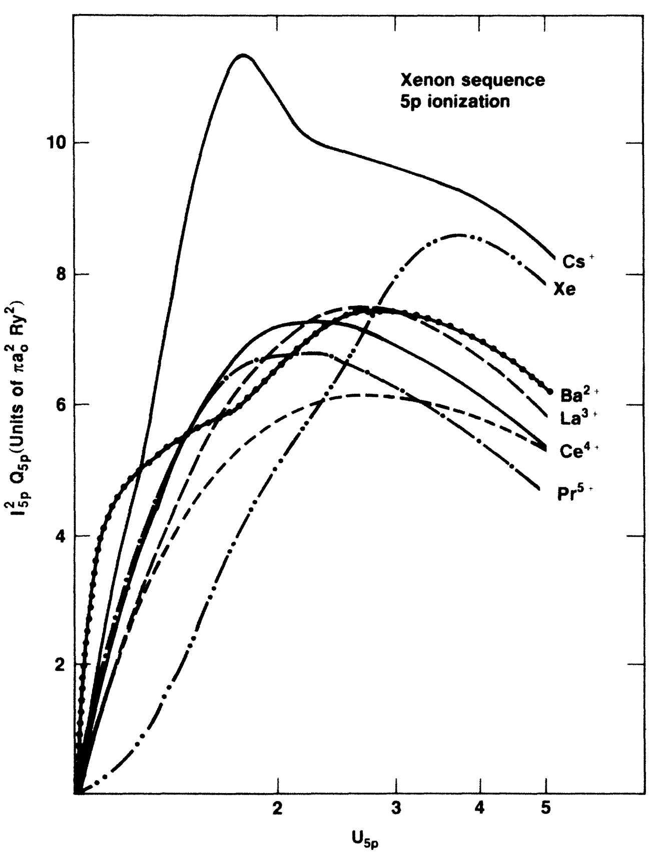

FIG. 3. Scaled electron impact-ionization cross sections for the $5p$ subshell of xenonlike ions computed in a distorted-wave Born-exchange approximation including the effects of scattering exchange and ground-state correlation.

continuum channels involved in the ionization of the $5p$ orbital of xenon can participate in shape resonances, there is no major feature in the cross section associated with any of them. Examination of the partial cross section as a function of the incident-electron partial-wave angular momentum shows that there is indeed a shape resonance in the incident channel at 1.0 a.u., but that it is masked by the contribution of the other partial waves in that channel. In the final state there is a complex interplay between the resonances in the scattered- and ejected-electron channels, with the result that the effects of both are washed out. Resonant behavior may be more apparent in more detailed examinations of the scattering process which include angular discrimination of the reaction products.

Experimental data for the single-electron-impact ionization of xenonlike ions in the ground state is available only for Xe (Ref. 21) and Cs^+ (Refs. 22 and 23). For Xe theory overestimates the observed cross section by more than a factor of 2. This poor agreement between theory and experiment for the Xe $5p$ cross section suggests that there are important additional interactions governing the cross section beyond the partial-wave term dependence and ground-state correlation included here. In an effort to identify the part of the calculation that is most important in defining the total cross section we performed a number of calculations using several different approximations for the partial-wave potentials. These approximations included: (1) The use of bound orbitals resulting from a Hartree-Fock approximation for the $Xe^-(5p^55d)$ negative ion to approximately account for the polarization of the target orbitals by the scattering electron, (2) description of the final target state by bound orbitals of the Xe^+ ion to partially account for relaxation of the target following ionization, (3) the use of a multiconfiguration approximation for the scattering potential including the effect of the $5p^45d^2$ excitation on the calculation of the partial waves, (4) calculation of all of the partial waves in the potential of the $5p^6$ ground state, as would follow from a straightforward application of perturbation theory in which all of the continuum orbitals are regarded as virtual excitations from the initial ground state, and (5) a plane-wave Born approximation in which the incident and scattered channels are represented by plane waves and the ejected channel is described by SCE distorted waves, shown by the x's in Fig. 1. Although these different approximations represent drastic modifications of the potentials used to determine the continuum waves, the effect on the $5p$ ionization cross section was only about $\pm 20\%$ at $u=4$, whereas the disagreement between theory and experiment is a factor of 2. Thus it would appear that the disagreement between theory and experiment for neutral xenon is due to some process more complex than can be represented by partial-wave potential modification.

Calculations of the neutral-xenon photoionization cross section using a term-dependent partial-wave approximation with ground-state correlation yield cross sections which are in general agreement with experiment, indicating that the description of the ejected channel by itself is reasonably appropriate, at least for the region of interaction space sampled by the dipole-interaction operator governing photon interactions. One might conjecture that the persistent disagreement of all of the distorted-wave approximations for the electron-ionization cross section with experiment is indicative of a more subtle rearrangement of the target-electron system than an essentially frozen-target approximation, such as the distorted-wave approximation can model. Interchannel coupling could result in a redistribution of the cross section among possible exit channels. Also, the triple resonance predicted for neutral xenon may not be adequately modeled by our simple distorted-wave approximation, and partial-wave energy-dependent changes in the resonant structure may significantly alter the angular momentum and energy distributions of the partial-wave summations. Consideration of target polarization by the incident wave, and the resulting self-consistent response of the free-electron channel to the modified target configuration, may be necessary to resolve the disagreement.

Poor agreement between theory and experiment has been found in previous calculations[24] for the electron-impact ionization cross sections of other rare-gas elements, notably Ar and Kr. It is interesting, however, that in the first ions of the respective isoelectronic sequences, K^+, Rb^+, and Cs^+, much closer agreement with experiment is achieved compared to the neutral atom. This is consistent with the concept of the asymptotic Coulomb field of the positive ions dominating the scattering event and making the cross sections much less sensitive to target-polarization effects. For Cs^+ theory overestimates the $5p$ ionization cross section by about 30%. There is some disagreement between the cross sections measured by Peart and Dolder[22] and by Hertling *et al.*[23] The later measurement indicates a much more pronounced feature at low incident electron energies which may be associated with the predicted shape resonance in the scattered wave channel. The effect of partial-wave term dependence on the Cs^+ $5p$ cross section is to raise the theoretical result, impairing agreement with both experimental curves. The addition of target-electron correlation compensates for this increase somewhat. Additional correlation may improve the agreement still further, although some holdover of the effects of target polarization discussed above for Xe is still expected to influence the ionization cross sections of Cs^+.

B. Ionization of the 4*d* subshell

Distorted-wave calculations of the cross sections for electron-impact ionization of the $4d$ subshell of Xe-Pr^{5+} are shown in Fig. 4. The same notation used in Fig. 1 is used to describe the results of different theoretical approximations for the $4d$ cross section. Experimental data is available for Xe and Cs^+. For neutral Xe we quote the recent measurement of Takayanagi *et al.*[25] for the $4d$

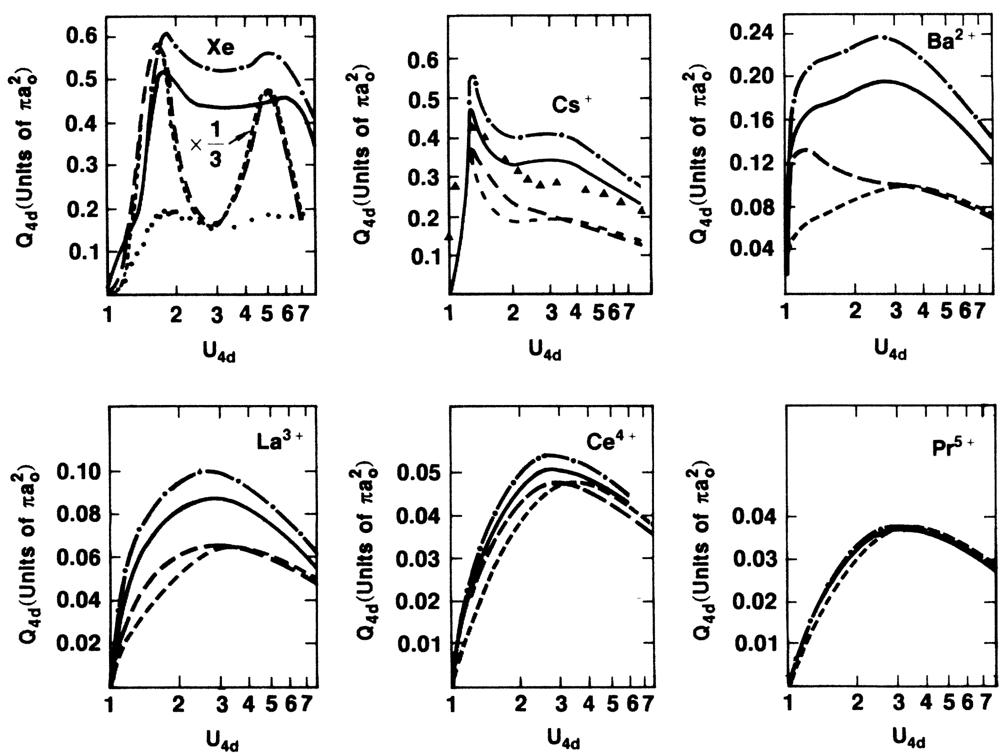

FIG. 4. Electron impact ionization cross sections for ionization of the $4d$ subshell of the first six members of the xenon isoelectronic sequence. -----, distorted-wave calculation without scattering exchange using SCE partial waves; — — —, distorted-wave Born-exchange approximation using SCE partial waves; —·—·—·, distorted-wave Born-exchange approximation using term-dependent kd-ejected partial waves; ——, distorted-wave Born-exchange approximation using term-dependent kd-ejected partial waves and including ground-state electron correlation. Experimental data: ●, Takayanagi *et al.* (Ref. 25); Δ, Hertling *et al.* (Ref. 23).

cross section, measured by the method of Auger electron spectroscopy. For Cs^+ we show the partial cross section for double ionization of the target.[23] The direct comparison of the present results with the measured double ionization cross section for Cs^+ is complicated by contributions to the latter including direct double ionization and excitation autodouble ionization. There has been as yet no quantum-mechanical study of the complex direct double-ionization process, and autodouble ionization is expected to be weak since it is a higher-order process. Previous studies[2] have shown, however, that $4d$ ionization followed by autoionization of the residual ion is a dominant contribution to the partial cross section for double ionization, especially for ionic targets. We therefore compare the measured cross section for double ionization with our calculations for $4d$ ionization, assume a unit branching ratio for Auger decay versus fluorescence, and remain cognizant of the possibility of additional contributions to the cross section due to direct double ionization and other higher-order processes.

For Xe and Cs^+ there are large contributions to the $4d$ cross section arising from shape resonances in the kf scattered wave channel. The origin and characteristics of these resonances have been discussed in detail in previous papers.[3,7,36] That they exert a more profound effect on the $4d$ cross section compared to the $5p$ or the $5s$ cross section is due to the increased importance of the kf scattered partial wave in determining the cross section of d orbitals.

Term dependence in the ejected kf channel has a major effect on both the shape and the magnitude of the $4d$ cross section. This is in accord with previous extensive studies of the photoionization cross section of the $4d$ subshell in xenonlike ions and other atoms and ions near the middle of the periodic table.[13,15,27,28] The large term-dependent exchange potentials in the wave equation for the kf ejected wave results in a "delayed maximum" in the photoionization cross section. At low ejected electron energy the partial wave does not penetrate the large repulsive potential barrier arising from exchange interactions with the $4d^9$ core. Overlap with the occupied orbitals remains small until electron energy increases sufficiently for orbital penetration to occur. At high ejected-electron energies significant cancellation occurs in the radial part of the transition matrix element, causing a reduction in the cross section. A similar phenomenon occurs in the electron scattering matrix element. The dependence of the scattering matrix element on the ejected electron energy is more complex, however, than in the case of photoionization. First, the interaction operator which links the bound and ejected orbitals consists of the electrostatic potential generated by the incident and scattered waves. This operator samples a different part of the bound-ejected wave overlap than the dipole operator which appears in the photoionization matrix element. Second, the requirement to conserve energy in the scattering event means that as the ejected energy changes so does the energy of the scattered wave, complicating the energy dependence of the scattering matrix element.

The effect of ground-state electron correlation on the cross section is similar for the $4d$ and $5p$ subshells. When term dependence is an important effect on the cross section, ground-state correlation in the initial target causes an almost uniform decrease in the cross section over the energy range considered here. For the higher ionization stages where term dependence grows progressively weaker, correlation effects are reduced also.

Figure 5 compares the scaled cross sections I^2Q computed in the Born-exchange approximation including term-dependent ejected partial waves and electron correlation in the initial target state. Complex electron interaction effects significantly affect the $4d$ cross section for only the first few ions of the sequence, beyond which a smooth asymptotic behavior is achieved.

IV. SUMMARY

We have performed a systematic study of the electron-impact ionization of the $5p$, $5s$, and $4d$ subshells of the first six members of the xenon isoelectronic sequence. The first few ions of the sequence were found to be sensitive to shape resonances in the scattered-electron channel, ejected-wave term dependence, and electron correlation in the initial target state. As the nuclear charge increases beyond $3+$, however, the strong central nuclear Coulomb potential begins to dominate the partial waves and the cross section. Agreement between the present results and experiment is poor for neutral xenon, and is of the order 25% for Cs^+, the only ion for which experimental data is currently available. Poor agreement for the neutral atom in the sequence is not unexpected for such a straightforward theoretical approximation to such

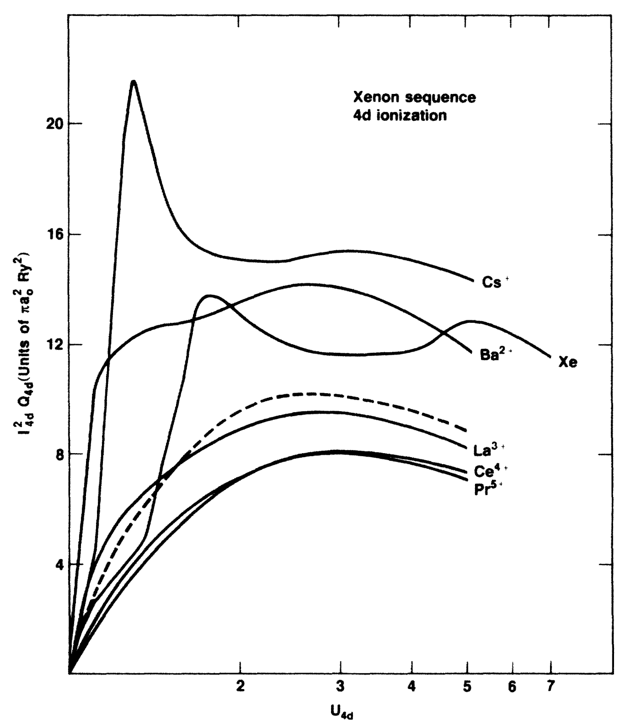

FIG. 5. Scaled electron-impact ionization cross sections for the $4d$ subshell of xenonlike ions computed in a distorted-wave Born-exchange approximation including the effects of scattering exchange and ground-state correlation.

a complex scattering event. Clearly more sophisticated calculations including the effect of the energy-dependent polarization of the target are required.

This study has concentrated on many-electron effects on the cross section for the direct electron-impact ionization of xenonlike ions. Also to be considered in a comparison of theory to experiment is the contribution of indirect mechanisms for ionization, most notably that of inner-shell excitation followed by autoionization. Such processes have been shown to be prominent features in the cross sections of ions containing a few valence electrons outside a high-electron-number subshell. In the xenon sequence one might expect transitions such as $4d^{10}5s^25p^6$-$4d^95s^25p^6nl$, where $nl=4f,5d,6s,6p,\ldots$ to be candidates for excitation autoionization. Although we have not yet done explicit calculations of the cross sections associated with these ionization channels, we note that the available experimental data does not suggest that they are dominant mechanisms at least for the more weakly ionized ions. A special consideration may apply to the $4f$ excitation, in that the $4f$ orbital is uncollapsed for Xe and Cs^+ (it resides in the outer potential well and has a relatively small overlap with the $4d$ subshell), is partially collapsed for Ba^{2+}, and becomes progressively more collapsed at higher Z. The uncollapsed nature of the $4f$ orbital in Xe and Cs^+ implies that the cross section for excitation to such states will be small for these ions. In Ba^{2+} a rough calculation of the threshold cross section was obtained using the effective-Gaunt-factor approximation,[29] with the result that the contribution of excitation followed by autoionization was about 5–10 % of the direct-ionization cross section. For more highly ionized atoms the contribution of the $4f$ excitations to the ionization cross section may be somewhat larger, owing to the stronger overlap of the $4d$ and $4f$ orbitals. A detailed analysis of such effects for the higher ionization states must include the increasing probability for the core excited states to radiatively decay rather than autoionize, and must also take account of the transition of the structure of the excited states to an intermediate coupling regime.

The present calculations are nonrelativistic, and it is important to understand what modifications relativistic effects could exert on the structure of the target and partial waves involved in the scattering event. It is known that for heavy atoms a contraction of the inner-shell orbitals due to direct relativistic effects results in increased screening of the outer subshell orbitals, which then expand to larger radii than nonrelativistic theory would predict. This expansion of the outer subshells in heavy ions can have an important effect on the formation of shape resonances in high angular momentum channels, since it can effectively move orbital charge density to the very region most significant in the formation of the intermediate potential barrier. This effect has been demonstrated in calculations of the $5d$ electron-impact ionization cross section of Fr^+ by Pindzola.[30] Relativistic effects on the scattering partial waves themselves are expected to be less significant in the determination of the cross section. This is because the electron ionization cross section is concentrated in the higher partial wave angular momenta, which are influenced less by relativistic effects than the more penetrating low angular momentum orbitals.

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