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GIANT RESONANCE PHENOMENA IN THE ELECTRON IMPACT IONIZATION OF HEAVY ATOMS AND IONS

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GIANT RESONANCE PHENOMENA IN THE ELECTRON IMPACT IONIZATION OF HEAVY ATOMS AND IONS

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INTRODUCTION

Heavy atoms and ions offer an interesting opportunity to study atomic physics in a region where the atomic structure is dominated by the interelectronic interactions. One illustration of this is the profound term dependence of atomic orbitals for certain configurations of heavy atoms and ions. This subject is extensively discussed elsewhere in the proceedings to this Institute. The present paper deals with another manifestation of resonance behavior, namely the appearance of giant scattering resonances in the cross sections for ionization of heavy atoms by electron impact. Such resonant structures arise from the double well nature of the scattering potential and have recently been identified in the cross sections for the electron impact ionization of several xenon-like ions.[1] In the present report, we summarize the results of calculations showing similar effects for a variety of other ions.

THEORETICAL METHOD

The electron impact ionization cross sections presented here were computed in a distorted wave Born exchange approximation. The target wavefunctions were represented by Hartree-Fock orbitals. The incident and scattered continuum electrons were computed in an approximation to the Hartree-Fock potential corresponding to the initial state of the atom or ion.[2] The $l=3$ ejected electron continuum orbitals were computed in a non-local term-dependent Hartree-Fock potential. For ionization of $4d^{10}$ subshells the $l=3$ ejected orbitals were computed in

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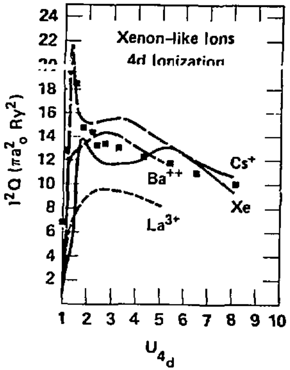

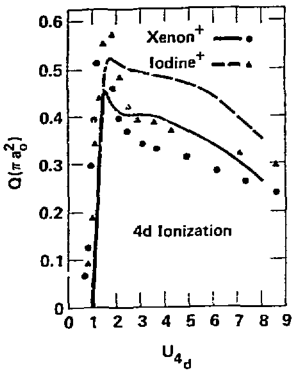

Figure 1. Scaled electron ionization cross section for xenon-like ions. Squares are the measurements of Hertling et. al.[6] for the double ionization of Cs^+ by a single electron impact.

Figure 2. Electron ionization cross sections for I^+ and Xe^+. The curves are distorted wave calculations and the points are the measurements of Achenbach et. al.[7].

term-independent approximate Hartree-Fock potentials. Sufficient partial waves were included in the triple partial wave expansion to ensure adequate convergence of the total cross section. Scattering exchange (exchange between the two final state continuum electrons) was included via the maximum interference theory of Peterkop[3]. In cases displaying very large resonance structures, the cross section was very sensitive to the method of integration over the final two-electron energy distribution. A 20 point Gauss integration was employed for this purpose. For ionization of $4d^{10}$ subshells, ground state correlation of the type $4d^{10}+4d^8 4f^2$ is included.[4] Further details of the computational methods used can be found in previous publications.[5]

EXAMPLES OF GIANT RESONANCES IN HEAVY ATOMS AND IONS

Xenon-like Ions: 4d Subshell Ionization

Ionization of a 4d electron in xenon-like ions leaves the residual ion in a singly autoionizing state, so that the 4d cross section contributes to effective double ionization of the target by a single electron impact. Figure 1 shows the scaled 4d electron ionization cross

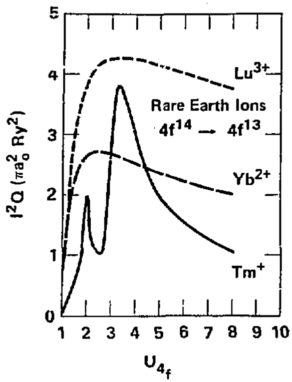

Figure 3. Scaled distorted wave electron ionization cross sections for the 4f ^{14} configuration in several rare earth ions.

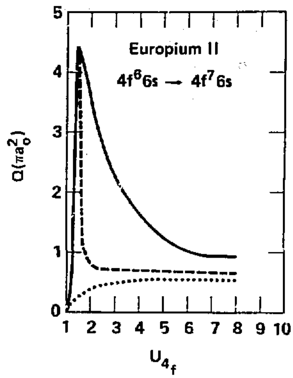

Figure 4. Scaled distorted wave electron ionization cross section for the 4f subshell in Eu^+. Solid curve: distorted wave Born-exchange; dashed curve: distorted wave without scattering exchange; dotted curve: Coulomb-Born without scattering exchange.

sections, I^2Q, for Xe, Cs^+, Ba^{++}, and La^{3+} vs. incident electron energy. In this paper, the cross section, Q, is given in units of πa_0 the ionization energy, I, is given in Rydbergs, and the incident electron energy is expressed in ionization threshold units, i.e., u=E/I where E is the continuum energy and I is the ionization energy. In Cs^+, the resonance is narrower and much more pronounced than in Xe and occurs at lower incident electron energy, as does the normal maximum. For Ba^{++}, the resonance occurs just above threshold, resulting in a very rapid rise in the cross section at low electron energies. For La^{3+}, the resonance disappears from the continuum and only the "background" cross section remains. Figure 1 also compares the present results for Cs^+ with the measurement of Hertling et al. Very good agreement is obtained both for to the shape of the resonance and the amplitude of the total cross section. It has been shown[1] that the phase shift of the l=3 scattered partial wave undergoes a phase shift of more than pi at approximately 1 Rydberg, coincident with the appearance of the resonance in the cross section. The resonance structure thus represents a true scattering resonance rather than a manifestation of term-dependence in the ejected electron continuum.

Xenon$^{\pm}$ and Iodine$^{\pm}$

Figure 2 compares our theoretical results for Xe^{+} and I^{+} with the measurements of Achenbach et. al.[7] In this case, the theory underestimates the amplitude of the resonant enhancement of the cross section at low incident energies. We note, however, that calculations done using configuration-averaged ejected f-waves show a much larger resonant enhancement than is observed, so it is possible that the present method over-corrects for the effects of ejected orbital term-dependence and correlation.

Ionization of the $4f^{14}$ Configuration

Figure 3 plots the cross sections for ionization of the $4f^{14}$ closed subshell of Tm^{+}, Yb^{++}, and Lu^{3+}. In this configuration, significant resonant behavior is found only for Tm^{+}. Preliminary studies done with term-dependent ejected f-waves ($4f^{13}kf\ ^{1}S$ channel) indicate that the second maximum in Tm^{+} is significantly reduced and broadened by ejected channel effects. The resonance at u=2 remains, however, and corresponds to a resonance in the scattered electron channel. Distorted wave calculations were done for 4f ionization from W^{+} and Hg^{+} to determine if the resonance reappeared when additional screening electrons were present. Neither of these elements was found to exhibit strong resonant behavior.

Europium^{+} $4f^{7}6s$ - $4f^{6}6s$ Configuration

Figure 4 presents cross sections for ionization of a 4f electrons from the ground configuration of Eu^{+}. A prominent resonant structure occurs at approximately 1.5 threshold units. The effect of scattering exchange is to broaden the resonance to higher energies, compared to the relatively narrow structure found when scattering exchange (exchange between the two final state continuum electrons) is neglected. Also shown in Figure 4 are the results of a Coulomb-Born calculation where the incident and scattered partial waves were computed in a Z=1 Coulomb potential and the ejected waves in a distorted wave potential. The Coulomb-Born approximation represents an approximate "background" cross section with which the full distorted wave cross section may be compared. Note that the effect of the resonance in the distorted wave calculation is to increase the low energy cross section by more than an order of magnitude over the "background" value.

SUMMARY

Distorted wave Born exchange calculations have revealed the presence of giant scattering resonances associated with the electron impact ionization of heavy atoms and ions. These resonances occur in the scattered electron channel, implying that they may serve as sensitive probes of the final state continuum-continuum electron interaction. Considering the complexity of such processes in heavy atoms the theoretical cross sections agree quite favorably with available experimental data. Additional calculations are in progress to further examine the nature of giant scattering resonances in electron ionization as well as other inelastic electron-ion processes.

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