Giant Resonances in the Electron-Impact Ionization of Heavy Atoms and Ions

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The first interpretation of giant resonance behavior in the inelastic scattering of electrons from heavy ions is reported for the electron-impact double ionization of Cs^+. A discussion of the partial-wave potentials and phase shifts leading to this phenomenon is presented along with results of several distorted-wave calculations of the cross section. The theoretical cross sections are in good agreement with the results of a crossed-beam measurement.

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Giant resonances in heavy atoms and ions have been shown to have a profound effect on the photoabsorption spectra of heavy atoms and ions.[1,2] Much of the theoretical and experimental work done on this subject has concentrated on the term dependence of core-excited states of the form d^9f. The strong exchange potential occurring between the f electron and the d^9 core results in an effective double-well potential[3] and properties associated with the bound nf and continuum kf states of such configurations depend critically on the degree to which the orbital penetrates into the inner well in which the bound core orbitals reside.[4] The term "giant resonance" has come to be applied to almost any excited orbital which exhibits pronounced term dependence, even if the strict conditions for resonance behavior (phase shift increase by π, addition of a node to the orbital[5]) are not satisfied.

The present work describes the first calculation of a genuine giant resonance phenomena which occurs in the electron-impact excitation and ionization of heavy atoms and ions, namely, a shape resonance which occurs in the *scattering* channel. As an example of such resonance effects we describe calculations performed for the multiple ionization of singly ionized cesium, a process which proceeds via single ionization of the $4d$ subshell of the $KLM4s^24p^24d^{10}5s^25p^6$ xenonlike ground state followed by autoionization of the residual ion, i.e.,

$$4d^{10}5s^25p^6+e^- \rightarrow 4d^95s^25p^6+2e^-$$
$$\rightarrow 4d^{10}5s^25p^4+3e^- .$$

The branching ratio for autoionization of the intermediate state is assumed to be unity.

The calculations reported here employ a distorted-wave electron-impact–ionization formalism which has been described in detail in previous publications.[4,6] Briefly, the target atom or ion is described by a Hartree-Fock approximation and the partial waves describing the scattering event are computed in realistic distorted-wave potentials. The incident and scattered partial waves are computed in an approximation to the frozen-core Hartree-Fock potential of the initial state.[7] The ejected electron is computed in the nonlocal term-dependent Hartree-Fock potential corresponding to the $4d^9kf\,^1P$ channel. Ground-state correlation of the type $d^{10}+d^8f^2$ was included in the initial state. The maximum-interference exchange approximation of Peterkop[8] is used to account for electron exchange among the two final-state free electrons. All energies are given in atomic units (1 a.u. = 27.21 eV) and cross sections are given in units of πa_0^2 ($a_0 = 0.529\times10^{-8}$ cm).

From previous studies of photoabsorption[1,2] and electron scattering[3,7] in heavy atoms it is known that the kf channel is especially sensitive to the details of the partial-wave potential. Figure 1 illustrates the kf partial-wave phase shifts corresponding to the $4d^{10}kf$ incident and scattered waves and the $4d^9kf$ ejected waves in Cs^+. First, note the extreme term dependence of the ejected kf waves. Whereas the $4d^9kf$

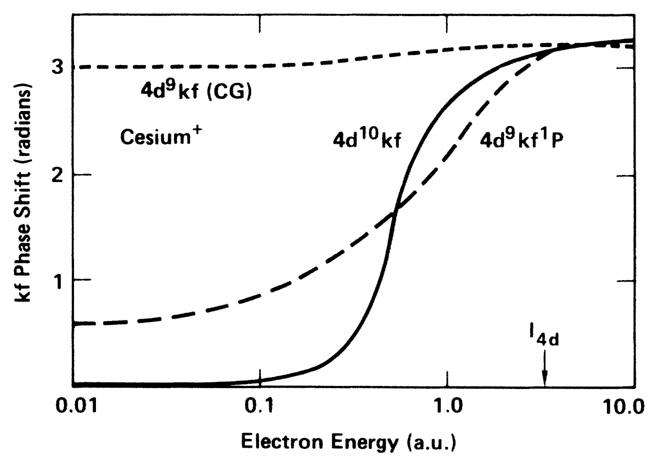

FIG. 1. Phase shifts for $l=3$ partial waves computed in the $4d^9kf$ center-of-gravity potential (dotted line), the $4d^9kf\,^1P$ term-dependent Hartree-Fock potential (dashed line), and the $4d^{10}kf$ potential (solid line). The dotted and dashed curves refer to approximations for the ejected electron; the solid curve, to the incident and scattered electron. Although the ejected channel exhibits pronounced term dependence, only the scattered wave undergoes a true resonance. Note that the threshold energy for ionization of a $4d$ electron occurs at too high an energy for the incident electron to participate in the shape resonance.

phase shift computed in the center-of-gravity Hartree-Fock potential is only weakly dependent on energy over the electron energy range from 0.01 to 10 a.u., the phase shift for kf waves computed in the term-dependent Hartree-Fock potential for the ^1P channel is small at low energy and rises only as the electron has sufficient energy to overcome the effects of the potential barrier separating the inner and outer potential wells. Even though the term dependence in the ejected channel is large, it does not constitute a giant resonance since the phase shift does not increase by π. Of even greater importance for the present study, however, is the true resonant behavior of the $4d^{10}kf$ channel. This is not a case of term dependence in the continuum, since this single optical electron channel has but one term. Rather, it is a manifestation of a shape resonance in the potential in which the continuum wave undergoes a phase shift of greater than π as the free-electron energy is increased.

Since the exchange interaction contributing to the potential is nonlocal and energy dependent, it is not possible to derive a single potential describing the scattering. In Fig. 2, however, we show the semiclassical exchange potential[7] (an excellent local simulation of the nonlocal Hartree-Fock potential) for a $4d^{10}kf$ electron with energy 0.41 a.u., illustrating the potential barrier separating the inner and outer wells. Also shown in Fig. 2 are scattered-channel kf partial waves corresponding to 0.22, 0.41, and 0.83 a.u. Note the addition of a node to the inner portion of the orbital as the continuum energy passes through the resonance.

Note that since the ionization energy of the $4d$ electron in Cs^+ is approximately 3.39 a.u., the incident kf electron involved in $4d$ ionization does not participate in the shape resonance. Only the lower-energy kf waves occurring in the scattered wave function are affected. This is especially exciting to the theorist in that it represents a critical test of theories relating to final-state continuum-continuum interactions in the complex electron-ionization event and is the first case found in which the description of the scattered orbitals plays a dominant role in determination of the cross section. This giant resonance will not be observed in photoabsorption experiments since the $4d^{10}kf$ channel does not couple radiatively to the cesiumlike ground state at energies compatible with resonant behavior of the orbitals.

Figure 3 presents theoretical cross sections for ionization of the $4d$ electron in Cs^+ computed in several different approximations. Also shown are the crossed-beam measurements of Hertling *et al.*[9] for double ionization via a single electron impact. The solid curve represents the most sophisticated approxi-

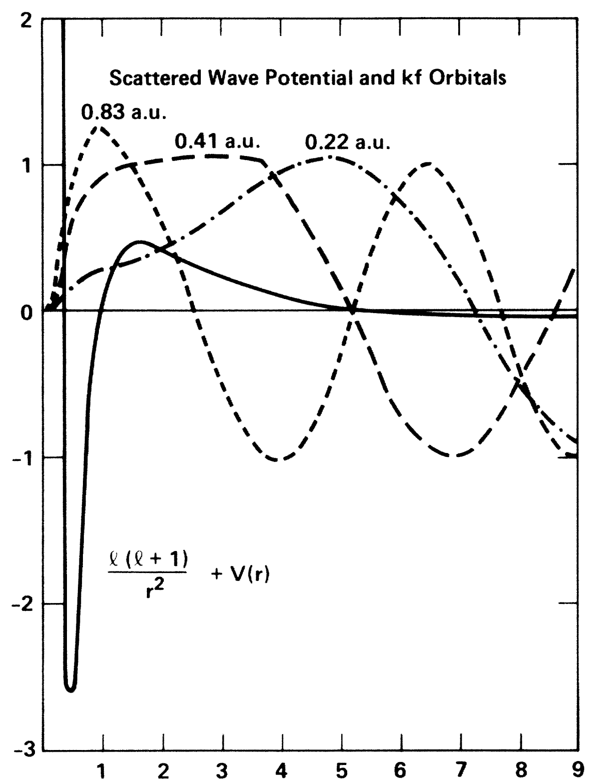

FIG. 2. Solid curve: local approximation for the potential (in atomic units) for f waves in the $4d^{10}kf$ configuration in Cs^+, illustrating the barrier separating the inner and outer potentials. Dashed curves: $l=3$ continuum orbitals computed in this potential normalized to unit asymptotic amplitude. Note the addition of a node to the orbital as the energy passes through the resonance.

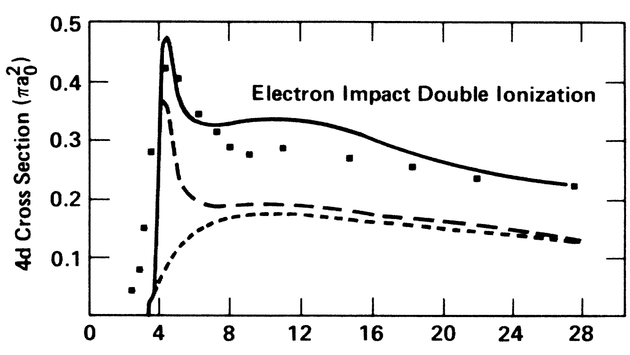

FIG. 3. Cross sections for ionization of a $4d$ electron in Cs^+, leading to autoionization of the final state and hence double ionization of the target by a single electron impact. Solid curve: distorted-wave Born exchange approximation using term-dependent Hartree-Fock ejected f waves and including ground-state correlation. Dashed curve: distorted-wave Born (no exchange) approximation using center-of-gravity ejected f waves. Dotted curve: Coulomb-Born (no exchange) approximation using center-of-gravity ejected f waves. Squares: crossed-beam experiment of Hertling *et al.* (Ref. 9).

mation in which the incident and scattered waves are computed in the $4d^{10}kf$ distorted-wave potentials and the ejected electron in the $4d^9kf\,^1P$ term-dependent Hartree-Fock potential. The cross section undergoes a very rapid rise at low electron energy as the scattered electron traverses the shape resonance. At approximately 8.5 a.u. the resonance is decaying and a local minimum in the cross section occurs. The normal (nonresonant) cross-section maximum is reached at 13.5 a.u. The agreement with experiments is excellent both in the shape and in the amplitude of the cross section.

In order to highlight the term dependence of the ejected partial waves as well as the association of the giant resonance with the scattered electron channel, we present in Fig. 3 the results of two other calculations of the $4d$ cross section. The dashed curved corresponds to another distorted-wave calculation where the ejected waves are computed in an approximation to the Hartree-Fock center-of-gravity potential. The dotted curve represents a Coulomb-Born calculation[6] in which the incident and scattered partial waves were described by $Z=1$ Coulomb waves (no potential distortion due to target electrons and hence no possibility of a shape resonance) and in which the ejected waves were identical to those used to compute the dashed curve. Neither the dashed nor dotted curves include ground-state correlation or scattering exchange so that they represent a direct comparison of the effects of the scattering potential on the cross section. A comparison of the dashed and dotted curves illustrates that the resonance only occurs when the distorted-wave potential is used. Comparing the two distorted-wave approximations, one with center-of-gravity–potential f waves (dashed curve) and one with term-dependent Hartree-Fock f waves (solid curve), one observes that although the amplitude of the cross section is sensitive to the details of the ejected orbitals, the resonance is a result of the scattering states and not the bound or ejected channels.

The giant resonance in the electron-impact double ionization of Cs^+ is the first reported interpretation of a giant resonance in the inelastic scattering of electrons from heavy ions. It was found in the course of a general study of electron ionization in ions of the xenon isoelectronic sequence, other results of which will be reported separately. Resonant behavior in the ionization of the $4d$ subshell has also been found for neutral Xe and for Ba^{++} and it is likely that it will occur for atoms and ions in other isoelectronic sequences as well.

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