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Merging of positions of zeros in dipole and quadrupole matrix elements of photoeffect from outer-shell and Rydberg states of high-Z elements

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The zeros in dipole and quadrupole matrix elements of photoeffect from the $ns_{1/2}$ subshells of uranium approach common positions as $n \rightarrow \infty$. This is an illustration of the more general feature that for sufficiently large n_0 photoeffect cross sections and angular distributions from nJL subshells, aside from the bound-state normalization factor which scales the cross section, are the same for all $n > n_0$ (J,L fixed) except for energies very close to threshold. This behavior can be expected for all subshells and all elements and for all multipole matrix elements.

In this paper we examine the position of zeros in dipole and quadrupole matrix elements, for photoionization from the $ns_{1/2}$ subshells of uranium in its ground state or excited states, as a function of principal quantum number n. Recent theoretical work shows that the quadrupole matrix elements can have a significant contribution to the low energy and x-ray photoelectron angular distribution,[1-3] while the dipole matrix elements dominate the total cross section in the same energy region. The existence of zeros in the dipole and quadrupole matrix elements has important consequences for photoeffect,[3-10] particularly in angular distributions[3,6-9] and subshell branching ratios,[10] which can be more dramatic than the changes in total cross sections. Multiple zeros in dipole ($nd \rightarrow \epsilon f$) matrix elements of excited atoms[11-13] and relativistic effects in the splitting and shifting of zeros in dipole matrix elements[14] have been reported. Multiple zeros also occur in screened potential quadrupole matrix elements for atoms in their ground state, and single zeros exist for quadrupole matrix elements even in the point Coulomb potential.

An interesting question is how the positions of these zeros (i.e., the energy for which the matrix element vanishes) varies as the principal quantum number n changes. Our study, based on a single-electron Dirac-Slater calculation for photoeffect from $ns_{1/2}$ subshells of uranium, indicates that the positions of zeros in dipole and quadrupole matrix elements become constant as $n \rightarrow \infty$. In our calculation the potential is fixed (calculated from ground-state configuration, imposing a Latter tail) as n varies through the shells of the ground state and then through successive outer shells of excited states with a common core; the features we are discussing should be independent of the particular choice of potential.[15] Our results are shown in Fig. 1, where the positions of zeros both in terms of photon energy and in terms of continuum photoelectron energy are plotted as a function of n.

The fixed position of zeros in matrix elements as $n \rightarrow \infty$ is due to the fact that as n increases the wave function (without the bound-state normalization factor) remains essentially unchanged except for its outermost lobe. This can be seen from Fig. 2, where the large component of various $ns_{1/2}$ bound-state wave functions (without bound-state normalization factor) of uranium are shown. Once n

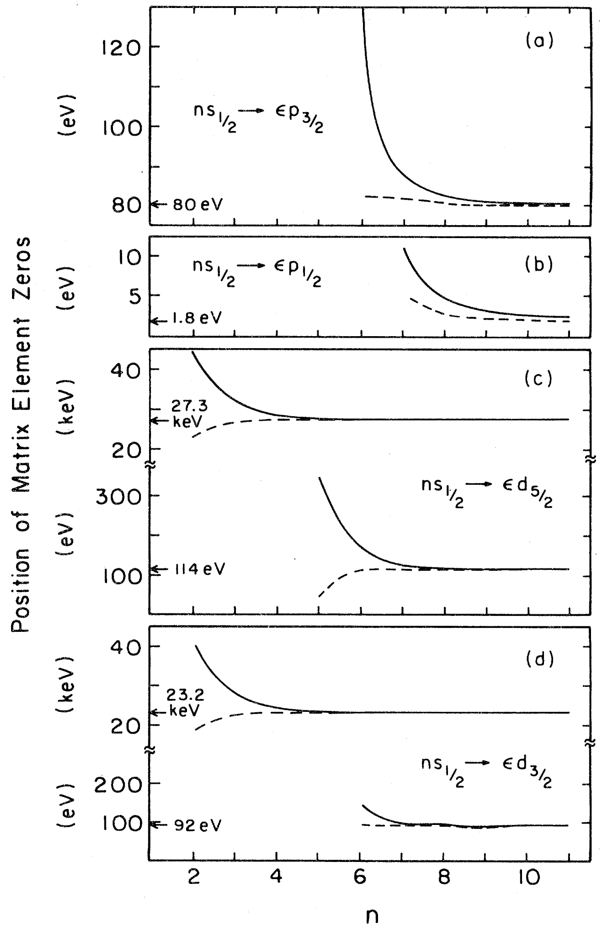

FIG. 1. Position of zeros in (a), (b) dipole and (c), (d) quadrupole matrix elements as a function of n for photoeffect from $ns_{1/2}$ subshells of uranium. The positions of zeros in matrix elements are expressed in terms of photon energy (solid line) and continuum photoelectron energy (dashed line). The arrow shows the position of the zero as $n \rightarrow \infty$. Note that we only have data for integers n, so that the smooth curves, drawn to aid the eye, are not to be taken seriously, particularly between $n = 5$ and 6 for the low-energy zero of (c).

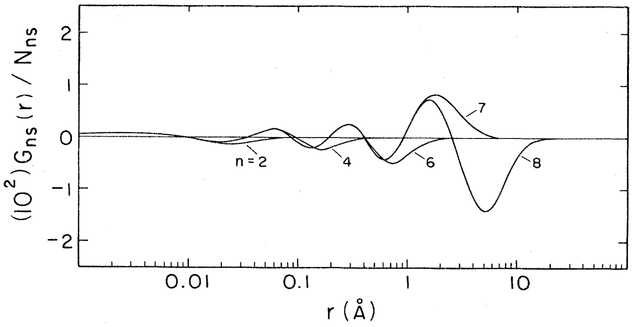

FIG. 2. Large component $[G_{ns}(r)]$ $(n=2,4,6,7,8)$ bound-state wave function [without normalization factor (N_{ns})] of uranium as a function of distance r (Å).

increases to a certain value n_0, for which that outermost lobe of the wave function does not contribute to the matrix element, the matrix element will essentially remain unchanged (for a fixed continuum energy) as n continues to increase. The outermost lobe for n_0, and the same lobe and others outside it for higher n, do not contribute to the matrix element because the continuum wave function is oscillating too rapidly (compared with bound-state wave functions), so that contributions from such distances average out to zero.

Thus one would more generally expect that at sufficiently high photoelectron energy, even for small n, values of matrix elements (again without bound-state normalization factors) at a given energy will merge to a common value, while values of matrix elements (without bound-state normalization factors) corresponding to large n will already merge at lower energies. This is indeed the case, as shown in Fig. 3. This feature had in fact previously been noted,[9] but it had not been appreciated that for sufficiently high n this would guarantee that the position of the Cooper minimum would stabilize. The above discussion also indicates that the continuum photoelectron energy is a better parameter to use than photon energy when comparing the matrix elements from different n (with the same J,L) in a fixed potential. This differs from other cases where photon energy is a better parameter than final electron energy, as in comparing the matrix elements in a screened Coulomb potential with point Coulomb matrix elements of the same initial states, or in the continuation of matrix elements from bound-bound to bound-free transitions.

Though our discussion here has used the example of the $ns_{1/2}$ subshells of uranium with a given potential, it should be a general feature for all multipole matrix elements, all subshells, all potentials, and all elements; the features are not restricted to the use of single-electron transition calculations.[15] As a consequence, for any given n_0 the photoeffect cross sections and angular distribution from nJL subshells, aside from the bound-state normalization factor, are the same for all $n > n_0$ (J,L fixed) for photoelectron energies greater than some specified value. Conversely, for any given photoelectron energy, there is an n_0 such that for $n > n_0$ the cross section and angular distribution are the same in the above sense.

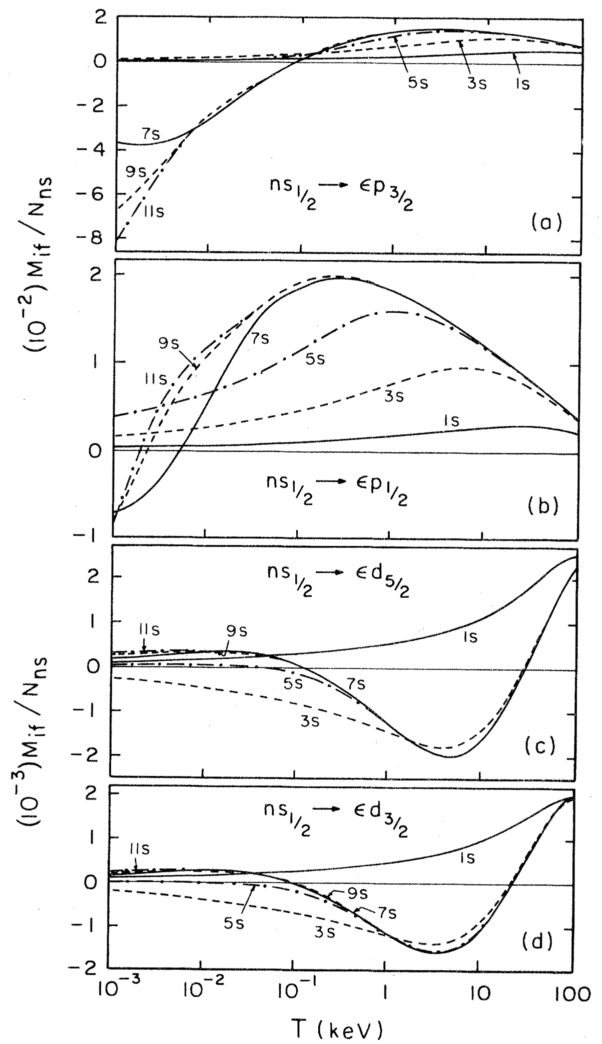

FIG. 3. (a), (b) Dipole and (c), (d) quadrupole matrix elements from $ns_{1/2}$ states of uranium (M_{if}/N_{ns}) as a function of photoelectron energy (keV).

It is also interesting to note the large relativistic splitting in Cooper minima which Fig. 1 illustrates. This had been discussed in Ref. 14 in connection with $6p$ photoionization; the data here attest to the universality of the phenomena and show that it also occurs in quadrupole transitions. The splitting between $6p_{3/2} \rightarrow \epsilon d_{3/2}$ and $6p_{3/2} \rightarrow \epsilon d_{5/2}$ was 28 eV, while here a 78 eV splitting is observed between $ns_{1/2} \rightarrow \epsilon p_{1/2}$ and $ns_{1/2} \rightarrow \epsilon p_{3/2}$. This reflects the decrease in the importance of the spin-orbit interaction with increasing angular momentum. The splitting of zeros for the quadrupole transitions $ns_{1/2} \rightarrow \epsilon d_{3/2}$ and $ns_{1/2} \rightarrow \epsilon d_{5/2}$ is 22 eV for the low-energy zero (which occurs at energies comparable to the dipole zero), and 4 keV for the high-energy zero. Note these splittings are scaling with the energy of the zero.

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[15] See Fig. 6 of M. Aymar, J. Phys. B 11, 1413 (1978). Their calculation shows that the position of the Cooper minimum in the photoeffect cross section from the *ns* state of sodium approaches a limit, a feature on which they did not comment.