CALCULATION OF PHOTOIONIZATION OF RELATIVISTIC ATOMS

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The calculations of photoionization cross section have faced two frequent problems. First, one frequently obtains different results for the so-named "length" and "velocity" formulations. That difference results from the two Hamiltonians used in the definitions of the bound and of the scattered electron states [1]. Secondly, relativistic corrections may become very important. Indeed, even for low energy photoelectrons and the top bound states, the asymmetry parameter β resulting from the Dirac equation may differ much from the one resulting from the Schroedinger equation. The photoionization cross section is written as

$$d\sigma/d\Omega = \frac{\sigma}{4\pi}(1 + \beta P_2(\cos\theta)) \qquad (1)$$

where the parameter β is associated with the $L = 2$ component of the spatial distribution. In the case of the Dirac equation, expressions for the cross section and the asymmetry parameter β were given by Walker and Waber [2].

The calculation of photoionization of relativistic atoms, which have large numbers of electrons, suggests using *density functional* procedures instead of *ab initio*. One uses one of its approximations such as LDA, LSD or GGA. We chose LDA in our calculations. Further, as shown by Da Costa et al [3], the use of pseudopotentials requires special cares because they break the equality between the "length" and the "velocity" results. Thus pseudopotentials are preferably to be avoided and the present calculation was all-electron.

Using LDA, the proper way to calculate the ionization potential and a single one-electron Hamiltonian for the scattered electron and for the bound state, thus making the velocity and length results equal, is very old and was named in the seventies as the "transition state". Its validity relies on a theorem formaly proven by Janak [4] as

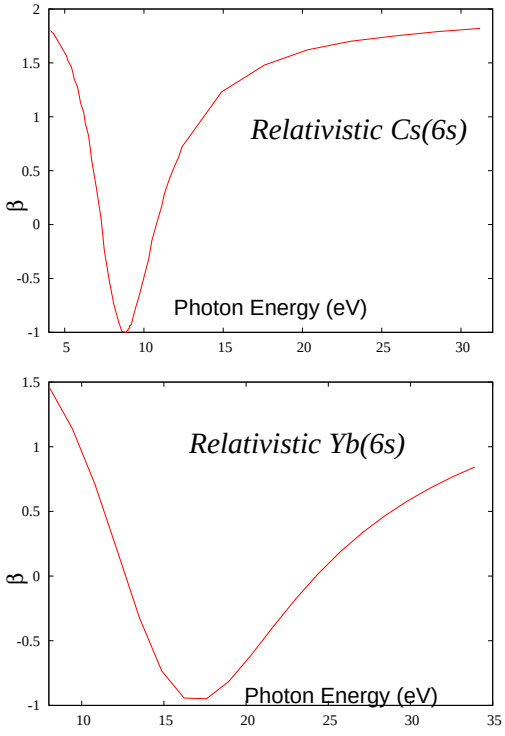
$$\frac{dE}{dn} = \epsilon \qquad (2)$$

where E is the total energy and ϵ is the Kohn-Sham one-electron eigenvalue. The transition state procedure consists of using the one-electron self-consistent Hamiltonian of the electron system with half electron removed.

In the following we present some results for the asymmetry parameter of the photoionization of the 6s electron of Cs and Yb. The calculated ionization potentials agree very well with experiment, a feature that is only possible with the transition state. The asymmetry parameter β deviates much from the non-relativistic value of 2, even for the highest occupied orbital 6s. Of course, the length and velocity calculations are the same.

First Ionization Potentials (eV)

Atom	Calculated	Experiment[5]
Yb	6.71	6.25
Cs	4.00	3.89



References

[1] D. Toffoli, M. J. Simpson, and R. R. Lucchese, Phys. Rev. A **69**, 062712 (2004).
[2] T. E. H. Walker and J. T. Waber, J. Phys. B: Atom. Molec. Phys. **6**, 1165 (1973).
[3] R. F. D. Costa, M. A. P. Lima, and L. G. Ferreira, Phys. Rev. A **67**, 052706 (2003).
[4] J. F. Janak, Phys. Rev. B **18**, 7165 (1978).
[5] EnvironmentalChemistry.com (2004).