Inner-shell photoionization of the beryllium isoelectronic sequence

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Time-dependent Hartree-Fock theory is used in conjunction with the Stieltjes imaging method to calculate the inner-shell photoionization cross sections of the beryllium isoelectronic sequence.

I. INTRODUCTION

The equations of time-dependent Hartree-Fock theory (TDHF) have been solved for several members of the beryllium isoelectronic sequence using numerical[1] and variational[2] methods. The numerical study provided oscillator strengths of the outer-shell transitions and for neutral beryllium the outer-shell photoionization cross section. The variational study provided oscillator strengths of inner- and outer-shell transitions, the results for the outer-shell transitions agreeing closely with the numerical solutions. Neutral beryllium has been investigated using the random-phase approximation[3] (RPA) and a comparison of the TDHF and RPA transition oscillator strengths of beryllium is presented in Table I. The values are in harmony as they should be since for closed-shell systems the two approximations have the same physical content.

Amusia *et al.*[3] also calculated inner- and outer-shell photoionization cross sections of beryllium, and their outer-shell cross sections agree closely with the numerical TDHF cross sections,[1] the remark to the contrary[3] arising seemingly from the different units employed.

In this paper we calculate inner-shell photoionization cross sections of the beryllium sequence by applying the method of Stieltjes imaging[4] to the variational study[2] and we use the RPA results of Amusia *et al.*[3] for beryllium to assess the validity of the procedure. The cross-section data are important in the description of the interaction of astrophysical x-ray sources with the ambient gas[5] and in the interpretation of high-temperature plasmas.[6]

TABLE I. Oscillator strengths of the transitions $1s^22s^21S$-$1s2s^2np$ and $1s^22s^2\,{}^1S$-$1s^22snp\,{}^1p$ of beryllium.

Final state	Oscillator strength TDHF [a,b]	RPA [c]
$1s2s^22p$	0.375	0.374
$3p$	0.035 2	0.035 4
$4p$	0.011 8	0.011 7
$1s^22s2p$	1.378	1.36
$3p$	0.022 7	0.023 2
$4p$	0.001 02	0.001 10

[a] Reference 1.
[b] Reference 2.
[c] Reference 3.

II. CALCULATIONS

The variational procedure for the solution of the TDHF equations has been described in detail.[2] It leads to a set of eigenvectors ϕ_i^1 and eigenfrequencies ω_i in terms of which the TDHF oscillator strength for a transition from an initial state with eigenvector ϕ^0 to a final state represented by ϕ_i^1 is given by

$$f_i = \tfrac{2}{3}\omega_i \left| \langle \phi^0 | \sum_{j=1}^{N} \vec{r}_j | \phi_i^1 \rangle \right|^2 ,$$

where $\vec{r}_j$ is the position vector of the jth electron of the N-electron atomic system and atomic units are used. Many of the states ϕ_i^1 have eigenfrequencies ω_i which locate them in the continuum. To obtain an estimate of the differential strengths we used the TDHF oscillator strengths and transition energies directly in the formula[4]

$$\left.\frac{df}{d\omega}\right|_{(\omega_i+\omega_{i+1})/2} = \frac{f_{i+1}+f_i}{2(\omega_{i+1}-\omega_i)} .$$

The values that we obtained with the simple formula are consistent with those given by the more-elaborate moment method,[4] which is usually of higher accuracy but yields fewer data points.

The TDHF and RPA cross sections for beryllium are compared in Fig. 1. The good agreement establishes the effectiveness of the discrete variational approach to the calculation of inner-shell photoionization cross sections within TDHF theory. Close-coupling calculations of the inner-shell photoionization cross sections of beryllium have been carried out by Bely-Dubau *et al.*[7] Their more-elaborate calculations take into account the interference between the discrete inner-shell excitations and the background continuum. At threshold, the close-coupling cross section is 1.6×10^{-18} cm^2, about 10% smaller than the TDHF

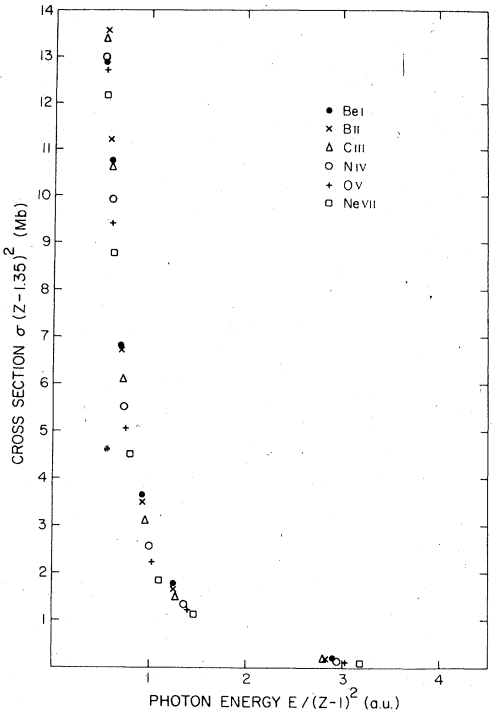

FIG. 1. Inner-shell photoionization cross sections $(Z-1.35)^2\sigma(\epsilon)$ in Mb as a function of $E/(Z-1)^2$ in a.u.

and RPA values.

The TDHF inner-shell cross sections for the beryllium sequence are shown in Fig. 2. Our calculations do not yield accurate ionization thresholds. At large Z, the ionization thresholds scale as $(Z-1)^2$ and in constructing Fig. 2 we assumed that the thresholds were located at $0.53(Z-1)^2$

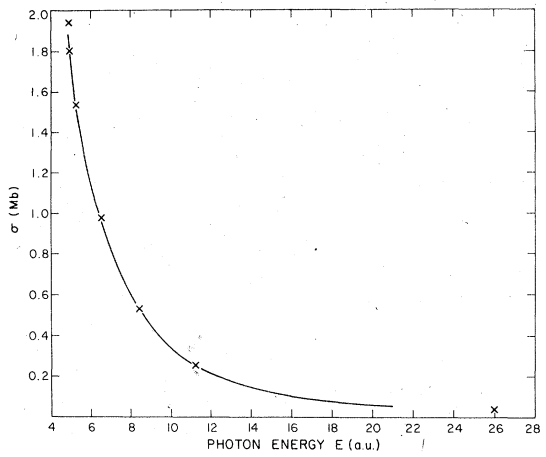

FIG. 3. Inner-shell photoionization cross sections of beryllium in Mb for photon energies E in a.u. (1 a.u. = 27.2 eV). The full curve is the RPA cross section calculated by Amusia *et al.* (Ref. 3). The X's are the Stieltjes imaging TDHF cross sections.

a.u., 4.73 a.u. being the TDHF threshold for beryllium. The experimental value for beryllium is 4.53 a.u.[8]

The cross sections $\sigma(E)$ are shown as a function of the energy E of the absorbed photon in atomic units in the form $(Z-1.35)^2\sigma(E)$, where Z is the nuclear charge. The screening model[9] suggests that σ should scale as $(Z-s)^{-2}$, where s is a screening parameter and a value somewhat larger than unity is physically plausible.

Because of perturbations due to the occurrence of pseudoresonances in a limited basis set, the imaging procedure failed for FVI. However, useful values for all Z can be obtained from a plot of

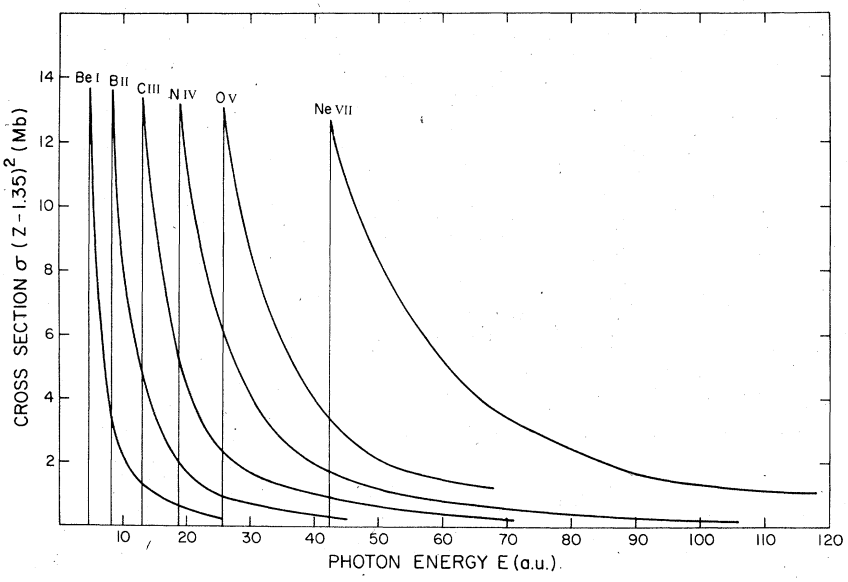

FIG. 2. Inner-shell photoionization cross sections $\sigma(E)$ in the form $(Z-1.35)^2 \times \sigma(\epsilon)$ in Mb for photon energies E in a.u.

$(Z-1.35)^2\sigma$ as a function of $E/(Z-1)^2$. Figure 3 presents this plot for the beryllium sequence.

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[1] R. F. Stewart, J. Phys. B 8, 1 (1975).

[2] R. F. Stewart, D. K. Watson, and A. Dalgarno, J. Chem. Phys. 63, 3222 (1975).

[3] M. Ya. Amusia, N. A. Cherepkov, Dj. Ziranovic, and V. Radojervic, Phys. Rev. A 13, 1466 (1976).

[4] P. L. Langhoff, Chem. Phys. Lett. 22, 60 (1973); P. L. Langhoff, S. R. Langhoff, and C. T. Corcoran, J. Chem. Phys. 67, 1722 (1977).

[5] S. Hatchett, J. Buff, and R. A. McCray, Astrophys. J. 206, 847 (1976).

[6] Cf. H. P. Furth, Nucl. Fusion 15, 487 (1977).

[7] F. Bely-Dubau, J. Dubau, and D. Petrini, J. Phys. B 10, 1613 (1977).

[8] G. Mehlman and J. M. Esteva, Astrophys. J. 188, 191 (1974).

[9] A. Dalgarno and E. M. Parkinson, Proc. R. Soc. A 301, 253 (1967).