Core polarization effect in the polarization cross section of atomic lithium

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Abstract   : The one-electron length form of the photoionization matrix element is used to compute the ground state phtoionization cross section of the atomic lithium The correction to the dipole transition moment due to core polarization is included. The behaviour of the computed photoionization cross sections near the threshold, is in agreement with earlier measurements and other reported calculations.

The importance of core polarization to study photoionization of atoms and ions has been emphasized earlier [1–7]. To account for the correlation of the outgoing electron with the core which exercises a very dominant effect on the nature of continuum wave function, such a correction is essential. According to McDowell [1], the effect of polarization of the core by the valence electron is small in the initial bound state, but appreciable in the final free state wave function. Weisheit and Dalgarno [2] computed the photoionization cross section for potassium with and without core polarization correction to matrix element and found that the photoionization cross sections with core polarization are orderly and almost coincident with experiment, while the same without such a correction are quite different. Tiwari *et al* [5] also studied the effect of polarization potential on the photoionization cross section of atomic Li but without taking into consideration the core polarization correction to matrix element and found an improvement over their previous calculation [8] without any such correction. Migdalek and Bojara [6] too have demonstrated the importance of core

polarization correction in the ionization potentials of *s*, *d* and *f* states of Rb and Cs isoelectronic sequences.

The working formula for the photoionization cross section is taken from the description given by McDowell [1] in the following form

$$a_v = 0.856 (I + K^2) \left| \int_0^\infty P_{kp}(r) Q(r) P_{2s}(r) dr \right|^2,$$ (1)

where *I* and K^2 are the ionization potential of the atomic Li and the kinetic energy of the photoelectron respectively (both given in *R*ydberg units). $P_{kp}(r)$ is the radial wave function for the continuum state and $P_{2s}(r)$ is the ground state radial wave function. The dipole length operator has been replaced here by the following corrected operator $Q(r)$ due to Weisheit [9].

$$Q(r) = r\left[1 - \frac{\alpha_d}{r^3} \left(1 - \exp - (r/r_c)^3 \right) \right]$$ (2)

The values of α_d and r_c for Li are taken from Table 1 of Hansen [7]. The normalized ground state wave function is adopted from the table of Roothaan *et al* [10] while the continua are numerically generated by solving the following Schrödinger equation in an independent particle (IPM) approximation [11].

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{2}{r^2} + V(r) \right] P_{kp}(r) = 0.$$ (3)

The static potential $V(r)$ in which the free state wave functions are constructed is the IPM potential of Szydlik and Green [12].

Eq. (3) is a second order linear differential equation with the first derivative absent and as such the Numerov procedure [13] has been invoked to numerically solve the eq. (3). In this procedure, $P_{kp}(r)$ is given as follows

$$P_{kp}(r+1) = \frac{1}{\left[12 - (\delta r)^2 F(r+1) \right]} \left\{ \left[24 + 10 (\delta r)^2 F(r) \right] \right.$$

$$\left. \times P_{kp}(r) - \left[12 - (\delta r)^2 F(r-1) \right] P_{kp}(r-1) \right\},$$ (4)

where $P_{kp}(r-1)$, $P_{kp}(r)$ and $P_{kp}(r+1)$ are the equally apart successively increasing values of the continuum wave function and $F(r-1)$, $F(r)$ and $F(r+1)$ are the similar three values of function $F(r)$. The function $F(r)$ is given by

$$F(r) = \frac{2}{r^2} - K^2 - V(r).$$ (5)

In order to get the next $P_{kp}(r)$, two initial values of $P_{kp}(r)$ are needed. This is obtained by considering the limiting form of the Schrödinger equation for $r \rightarrow 0$. When $r \rightarrow 0$, the Schrödinger equation may be approximated as

$$\frac{d^2}{dr^2} P_{kp}(r) = \frac{2}{r^2} P_{kp}(r) \qquad (6)$$

and this equation has the following trivial solution $P_{kp}(r) = $ constant. r^2.
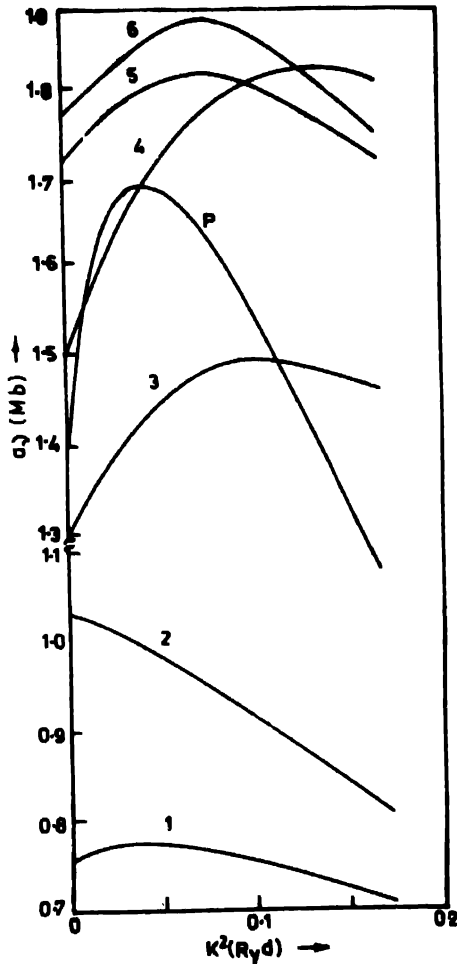

Figure 1. Photoionization cross section of Li.

1. Without polarization by Tiwari *et al* [8].
2. With polarization by Tiwari *et al* [15]
3. Hartree Fock calculation by Chang and McDowell[15] without polarization.
4. Experiment of Hudson and Carter [16].
5. The many body calculations of Chang and McDowell [15].
6. Hartree Fock results by McDowell and Chang [17] including polarization effect.
P. Present calculation.

The numerically generated continua are normalized by Stewart's [14] method. If the unnormalized solution initially achieved in the asymptotic region is written as $P'(r)$ such that

$$\frac{P'(r)}{N} = P(r),$$ (7)

where N is the normalization constant, then

$$N = 1/2 \left[\left(a_1 + a_2 \right)^2 \sec^2 \alpha + \left(a_1 - a_2 \right)^2 \mathrm{cosec}^2 \alpha \right]^{1/2},$$ (8)

where $\quad a_1 = \pi^{1/2} Z_1^{1/2} P'(r), \quad a_2 = \pi^{1/2} Z_2^{1/2} P'(r_2), \quad \alpha = \frac{1}{2} \int_{r_1}^{r_2} Z\, dr$

and $\quad Z^2 = \lambda - \frac{1}{\lambda}\left(\frac{1}{r^3} - \frac{3}{r^4} \right) + \frac{1.25}{\lambda^2}\left(\frac{2}{r^3} - \frac{1}{r^2} \right)^2$

with $\quad \lambda = k^2 - \frac{2}{r^2} + \frac{2}{r}.$

Special care is taken to avoid those values of α which are equal or even very close to $n\pi$ and $(2n+1)\pi/2$ where n is an integer. The integration involved in the normalization of continua is done by Gauss quadrature rule while the same involving the matrix element is accomplished using the Simpson quadrature rule. The starting value of the radial interval dr considered in the present calculation, is 10^{-6} Å. The computer program has been so designed and adjusted that the radial interval continues to be doubled each time per 2000 steps until a radial distance of about 32 Å is covered.

In Figure 1, the results are compared with the other reported calculations and also with similar calculations of Tiwari *et al* [5] but without core polarization correction. An improvement has been found especially at the low photon energies. The potential has however, been found not suitable at high energies.

Acknowledgment

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