Photoionization of He and Li^+

M. Daskhan
Department of Physics, Ramkrishna Mission College, Narendrapur, 24 Parganas, West Bengal, India

A. S. Ghosh
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India

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The continuous oscillator strengths and photoionization cross section of He and Li^+ are calculated by use of the polarized-orbital method. Matrix elements involving distorted-target wave functions have been included. The results are found to be in excellent agreement with the experimental values.

INTRODUCTION

We consider the photoionization of the He and the Li^+ ion. In our earlier paper,[1] we employed the polarized-orbital method (POM) to calculate the photodetachment cross section of H^-. Bell and Kingston[2] have also used the POM to obtain the continuum wave function. In our previous work,[1] we included the matrix elements involving target-distortion wave function, whereas Bell and Kingston have neglected these matrix elements. Our results for H^- are encouraging. In the present paper, we have extended our previous work to calculate the photoionization cross section of He and Li^+.

There are some reliable calculations[3-7] for the helium atom, and some of the results[3,4] are in very good agreement with the most recent experimental (West and Marr[8]) values. Information about the photoionization cross sections for the ionized member of the helium sequence are scanty. Apart from the Hartree-Fock calculations of Stewart and Webb,[9] Bell and Kingston[10,11] evaluated the cross sections using increasingly more accurate bound-state functions and the polarized-orbital free-state function. These results are in fair agreement with measured values.

The methods used in the case of He are elaborate and it is very difficult to extend these methods to complex systems. The method of polarized orbital is very simple in comparison with these elaborate methods. The present method can be applied to more complex systems without much trouble excluding those targets which have very high polarizability. Moreover, the importance of the matrix elements involving target-distortion wave function is well known for scattering calculations. Here we have calculated the free-state function following the method of Temkin and Lamkin[12] (p-wave correction is made by Sloan[13]). The effect of the exhange polarization has been included. The 20-parameter wave function of Hart and Herzberg[14] is used to represent the He atom and the Li^+ ion. The photoionization cross sections have been evaluated in the length form only.

THEORY

It is well known that the polarized orbital method (POM) takes into account the long-range polarization properly and fails to incorporate the short-range correlations. Now, the length formulation weighs on the large electron separations. Therefore the length formulation results are believed to be reliable for the polarized-orbital free-state functions. The continuous or differential oscillator strength per unit Rydberg energy in the continuum in the length form may be written as

$$\left(\frac{df}{d\epsilon}\right)_L = (I+\epsilon)\left|\int \Psi_d^*(\vec{r}_1+\vec{r}_2)\Psi_c(\epsilon)\,d\vec{r}_1 d\vec{r}_2\right|^2 , \qquad (1)$$

where a photon of energy $(I+\epsilon)$ is absorbed and an electron of energy ϵ is emitted by the system. We express energy in Rydberg units and all other quantities in atomic units. The wave functions Ψ_d and Ψ_c represent the initial and final states, respectively. Both the bound and free states are singlets and the nonzero contribution to the matrix elements comes from the p-wave part of the free-state wave function. The bound-state wave function used is the 20-parameter function of Hart and Herzberg.[14] In choosing the bound-state wave function of He and Li^+ we have been guided by the findings of Bell and Kingston. They found that the 20-parameter wave function is the adequate representation of the bound states of He and Li^+. The free-state wave function is determined by the method following Temkin and Lamkin[12] and Sloan.[13]

The photoionization cross section (σ) in Mb is given by

$$\sigma = 8.078\left(\frac{df}{d\epsilon}\right)_L , \qquad (2)$$

when the continuous oscillator strength is measured per unit Rydberg.

RESULTS AND DISCUSSION

Photoionization of He

We have solved the integro-differential equations using the method as employed by Temkin and Lamkin[12] and Sloan.[13] We have reproduced the phase shifts of Sloan as a check of our program by using a suitable step size. The photoionization cross section of helium in the photon energy region for 1.9 to 5.8 Ry are shown in Fig. 1 along with

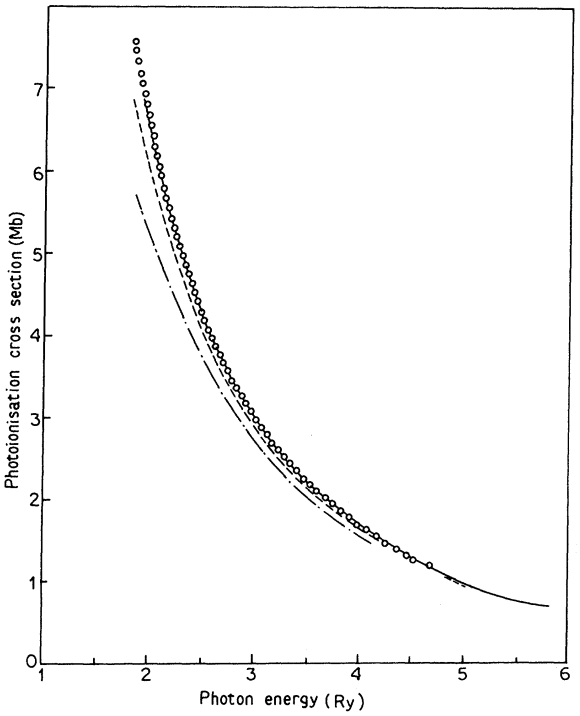

FIG. 1. Photoionization cross section for the transition $h\nu + \mathrm{He} \rightarrow e^- + \mathrm{He}^+$: ——, present results; — · — ·, three-state velocity of Berrington *et al.* (Ref. 3); — — —, six-state velocity of Berrington *et al.* (Ref. 3); OOO, experiment of West and Marr (Ref. 8).

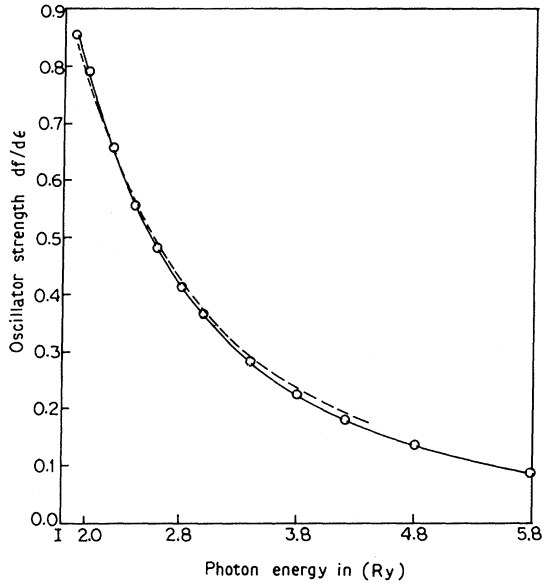

FIG. 2. Continuous oscillator strength for the transition $h\nu + \mathrm{He} \rightarrow e^- + \mathrm{He}^+$: ——, present results; — — —, Stewart (Ref. 4); OOO, West and Marr (Ref. 8).

the corresponding theoretical predictions in the velocity form by Berrington, Burke, Fon, and Taylor[3] using the three and six-state basis. The recent experimental values of West and Marr[8] have also been compared. Over the energy range considered the present results coalesce with the measured values. It may be mentioned that the six-state calculations in the length approximation by Berrington *et al.*[3] are almost indistinguishable on the scale of this figure. Therefore we could not plot the six-state length form results of Berrington *et al.* in the figure. In Fig. 2 we have given the results of continuous oscillator strength of He along with those of the elaborate calculation of Stewart.[4] The corresponding experimental predictions of West and Marr[8] have also been included. In both cases the results for He are very reliable. Numerical values of oscillator strength and photoionization cross section can be obtained from Tables I and II, respectively. Importance of the matrix elements involving the target-distortion wave function can be obtained

TABLE I. Comparison of the photoionization cross sections (σ) for the $1s^2\,{}^1S \rightarrow 1s\epsilon p\,{}^1P$ transition in helium; σ is given in Mb.

Photon energy $I+$ (Ry)	Present results with Φ^{pol}	Experiment West and Marr (Ref. 8)	Stewart (Ref. 4)
1.9	6.93	6.87	6.81
2.0	6.30	6.40	6.29
2.2	5.27	5.28	
2.3	4.84	4.87	4.98
2.4	4.67	4.51	
2.6	3.84	3.88	
2.8	3.33	3.36	3.48
3.0	3.02	2.98	
3.4	2.29	2.31	
3.6	2.05	2.07	
3.8	1.85	1.85	1.92
4.2	1.53	1.56	
4.8	1.13	1.13	
5.8	0.74	0.75	

TABLE II. Comparison of the oscillator strength $df/d\epsilon$ for the $1s^2\,{}^1S \rightarrow 1s\epsilon p\,{}^1P$ transition in helium.

Energy of ejected electron (Ry)	Polarized orbital present with Φ^{pol}	Polarized orbital Bell and Kingston (Ref. 8)	Close coupling Burke and McVicar (Ref. 7)	Experiment West and Marr (Ref. 8)	Stewart (Ref. 4)
0.1	0.858	0.867	. . .	0.851	0.843
0.2	0.780	0.803	0.778	0.793	0.779
0.4	0.653	0.689	0.668	0.654	
0.6	0.553	0.593	0.573	0.558	
0.8	0.475	0.514	0.499	0.480	
1.0	0.412	0.447	0.455	0.416	0.431
1.2	0.374	0.392	0.381	0.365	
1.6	0.283	0.306	0.298	0.286	
1.8	0.254	0.272	0.266	0.257	
2.0	0.229	0.243	0.240	0.229	0.236
2.4	0.189	0.197	0.200	0.193	
3.0	0.140	0.147		0.140	
4.0	0.090	0.0956		0.093	

from Table I. Our contention that the full polarized-orbital wave function should be used in the scattering calculations is correct.

Photoionization of Li^+

The results of oscillator strength for the photoionization of Li^+ are shown in Fig. 3 and Table III together with the corresponding theoretical values of Bell and Kingston.[10]

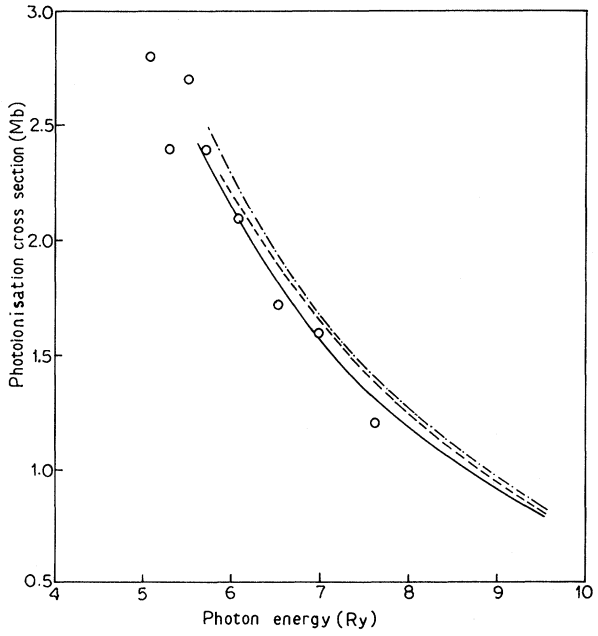

FIG. 3. Photoionization cross section for the transition $Li^+ + h\nu \rightarrow e^- + Li^{2+}$: ——, present results; – – –, Amusia *et al.* (Ref. 16); – · – ·, Bell and Kingston (Ref. 10); ooo, experiment of Mehlman *et al.* (Ref. 15) on the K-shell photoionization of the lithium atom.

Since the outer electron of atomic lithium is rather weakly bound, we might expect that at high photon energies the photoionization cross section for atomic lithium would not differ greatly from that of Li^+. For this reason, we have included in Fig. 3 the very recent experimentally measured photoabsorption cross-section values of the K shell of the atomic lithium by Mehlman, Copper, and Saloman[15] and the theoretical results of Amusia *et al.*[16] The results of Bell and Kingston, who have neglected the matrix element involving distorted-target wave function, and of Amusia, Cherepkov, Zivanovic, and Radojevic, who have employed random-phase approximation with exchange lie above our theoretical predictions in the given energy range. The present photoionization cross sections are found to be in best agreement with the measured values.

TABLE III. The continuous oscillator strength $df/d\epsilon$ of Li^+ calculated with use of a 20-parameter ground-state wave function and a polarized-orbital free-state wave function in the dipole length formulation.

Energy of ejected electron (Ry)	Present results including Φ^{pol}	Bell and Kingston (Ref. 10)
0.2	0.2863	0.3090
0.6	0.2514	0.2706
1.0	0.224	0.2381
1.4	0.1985	0.2105
1.6	0.1782	0.1982
2.0	0.1607	0.1762
2.4	0.1508	0.1574
2.6	0.1450	0.1489
3.0	0.1281	0.1337
4.0	0.0952	0.1037

CONCLUSION

We conclude that the polarized-orbital method is reliable in predicting the photoionization cross section at least for the helium and heliumlike ions. This method reproduces the results that have been obtained by use of the very elaborate theoretical calculations. Depending on the simplicity and the physical feature, this method may be used for the complex systems.

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