DOE/ER/02892--28

DE82 006913

CONF-800626--10

Paper Presented at the VI International Conference on Vacuum Ultraviolet Radiation Physics, Charlottesville, Virginia, 2-6 June 1980, Extended Abstract No. II-58.

COO-2892-28

PHOTOIONIZATION CROSS SECTION FOR He IN THE HYPERSPHERICAL COORDINATE METHOD

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In order to more fully explore the role of electron correlations in the photoionization process, we have employed the hyperspherical coordinate method of Macek[1] in calculating photoionization cross sections of He. While this system of coordinates has long been recognized as particularly suitable for the description of two-electron dynamics[2] it is only recently that quantitative calculations have been made. Previous applications have included predictions of doubly-excited-state energies in He and H^-,[1,3-5] and the treatment of two-electron atomic scattering.[3,6] Ours is the first application of the method to a dipole process.

The hyperspherical coordinate system expresses the six-dimensional two-electron space in terms of a hyperspherical radius $R = (r_1^2 + r_2^2)^{\frac{1}{2}}$ and five angular variables. Following Macek,[1] we take these to be $\alpha = \mathrm{Tan}^{-1}(r_2/r_1)$, $\hat{r}_1$ and $\hat{r}_2$. In this set of coordinates, the two-electron Schrödinger equation is nearly separable. The wavefunction is written as

$$\Psi(R,\alpha,\hat{r}_1,\hat{r}_2) = (R^{5/2}\sin\alpha\cos\alpha)^{-1}\sum_u F_u^{(R)}\phi_u(R;\alpha,\hat{r}_1,\hat{r}_2). \qquad (1)$$

The eigenvalues of the angular equation, which are parametrically dependent upon R, yield channel potentials for the radial equation, and the eigenfunctions, ϕ_u, of the angular equation are used to obtain the channel-channel coupling for the radial equation.

Our first application of the hyperspherical method has been to calculate cross sections for photoionization of He using a single-channel, adiabatic approach, from threshold to 1 a.u. above threshold. In this energy range the residual ion is in its ground state. Our initial (final) -state wavefunction was obtained by using the lowest $^1S^e(^1P^o)$ potential curve along with the diagonal coupling-matrix element in the radial equation. As a measure of the degree of correlation contained in our wavefunctions, we observe that our ground state

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energy (-2.89517 a.u.) is quite close to the essentially exact result of Pekeris[7] (-2.90372 a.u.) in comparison with the Hartree-Fock[8] ground state energy (-2.86168 a.u.).

In Table 1 we compare our cross section results with those of other detailed calculations[9-11] as well as with revised experimental data of Samson,[12] which have error bars of ± 3%. Within the kinetic energy range $0.0 \leq \varepsilon \leq 0.25$ a.u. our results are comparable to or slightly better than these other calculations. Above $\varepsilon = 2.5$ a.u. the RPA[9] and polarized orbital[11] calculations tend higher than experiment, while our results tend lower (≈12% lower at $\varepsilon = .9$ a.u.). Close-coupling results[10] are not given below $\varepsilon = 0.1$ a.u. because of numerical problems near threshold, but above $\varepsilon = 0.25$ a.u. they are in best agreement with experiment. Preliminary calculations indicate that when the hyperspherical channel corresponding to the n = 2+ state is included the cross section is practically unchanged near threshold, but is increased by about 10% over the single channel result at $\varepsilon = 0.9$ a.u.

Table 1. Comparison of the Present Results with Some of the More Detailed Theoretical Calculations of the Photoionization Cross Section for the Process $He + \omega \rightarrow He^+(1s) + e^-$

	σ(Mb)[b]				
Photoelectron Energy(a.u.)[a]	Experimental results[c]	Present results[d]	RPA Method[e]	Close-Coupling Method[f]	Polarized Orbital Method[g]
0.0	7.56 ± 0.23	7.65	7.55	——	7.56 (7.84)
0.05	6.89 ± 0.21	6.96	7.00	——	7.00 (7.24)
0.1	6.41 ± 0.19	6.36	6.45	6.32 (6.25)	6.47 (6.69)
0.15	5.92 ± 0.18	5.81	6.00	——	——
0.2	5.52 ± 0.17	5.33	5.55	5.38 (5.34)	5.55 (5.72)
0.25	5.02 ± 0.15	4.88	5.18	——	——
0.3	4.63 ± 0.14	4.48	4.85	4.61 (4.59)	4.79 (4.92)
0.4	3.94 ± 0.12	3.81	4.28	3.98 (3.97)	4.14 (4.25)
0.5	3.41 ± 0.10	3.26	3.75	3.47 (3.46)	3.61 (3.70)
0.7	2.57 ± 0.08	2.43	2.87	2.68 (2.67)	2.79 (2.85)
0.9	2.10 ± 0.06	1.85	2.23	2.13 (2.11)	2.19 (2.23)

[a] 1 a.u. = 27.2108 eV. [b] Theoretical results are given in dipole length approximation. When available, dipole velocity results are given in parenthesis. [c] Ref. 12. Linear interpolation of the densely spaced experimental results (see Fig. 1) is used to provide values at the same energies for which theoretical

results are available. [d]The diagonal non-adiabatic coupling terms are included in calculating both initial and final state wavefunctions. [e]Ref. 9. Numerical values were supplied to us by the author. [f]Ref. 10, Table IV. Final state is obtained from a $1s - 2\bar{s} - 2\bar{p}$ expansion. Initial state is the 56-term Pekeris variational wavefunction. [g]Ref. 11, Table 2. Initial state is the 2-term Hart-Herzberg variational wavefunction.

This work was supported in part by U.S. Department of Energy Contract No. EY-76-S-02-2892. Support of AFS by an Alexander von Humbolt Research Fellowship is gratefully acknowledged.

REFERENCES

1. J. Macek, J. Phys. B 1, 831 (1968).
2. See e.g. P. M. Morse and H. Feshback, Methods of Theoretical Physics, Part II, (McGraw-Hill, New York, 1953), pp. 1729-34.
3. (a) U. Fano, Atomic Physics 1 (Plenum, New York, 1969) pp. 209-225; (b) U. Fano and C. D. Lin, Atomic Physics 4 (Plenum, New York, 1975), pp. 47-70; (c) C. D. Lin, Phys. Rev. A 10, 1986 (1974); (d) Phys. Rev. Lett. 35, 1150 (1975).
4. (a) H. Klar, J. Phys. B 7, L436 (1974); (b) M. Klar, Doctoral Thesis (1977), Fakultät für Physik der Albert Ludwigs Universität, Freiburg, West Germany (unpublished); (c) H. Klar and M. Klar, J. Phys. B (in press).
5. C. Greene, J. Phys. B 13, L39 (1980).
6. C. D. Lin, Phys. Rev. A 12, 493 (1975).
7. C. L. Pekeris, Phys. Rev. 112, 1649 (1958).
8. E. Clementi and C. Roetti, At. Data and Nucl. Data Tables 14, 177 (1974).
9. G. Wendin, Phys. Lett. 33A, 16 (1970); J. Phys. B 4, 1080 (1971).
10. V. Jacobs, Phys. Rev. A 3, 289 (1971).
11. K. L. Bell and A. E. Kingston, Proc. Phys. Soc. 90, 31 (1967).
12. J. A. R. Samson, Phys. Reports 28C, 303 (1976).

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