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LETTER TO THE EDITOR

Photoionization cross section for He in the hyperspherical coordinate method

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Abstract

The hyperspherical coordinate method developed by Macek, Fano, Lin, and Klar to describe two-electron correlations is used for the first time to treat an atomic photoionization process. Using adiabatic approximations for both the initial and the final state, the cross section for the process $\text{He} + \gamma \rightarrow \text{He}^+1s + e^-$ is calculated and is found to lie 1% higher than the revised experimental data of Samson at threshold, 4% lower at 1 Ryd above threshold, and 12% lower at 1.9 Ryd above threshold.

While the use of hyperspherical coordinates to describe two-electron correlations is quite old (Morse and Feshbach 1953, Smith 1960, Macek 1967), it is only relatively recently that Macek (1968) introduced an adiabatic approximation in such coordinates which provided quantitatively accurate predictions of doubly-excited-state energies in He as well as a good description of two-electron dynamics. Further development of the theory and numerous applications to doubly excited states of He and H^- have been made by Fano and Lin (Fano 1969; Fano and Lin 1975; Lin 1974, 1975a), H. Klar and M. Klar (H. Klar 1974; M. Klar 1977; H. Klar and M. Klar 1980) and Greene (1980). Application of the method to treat two-electron atomic scattering processes have been described by Fano (1969) and by Fano and Lin (1975), but only the ^1S electron-hydrogen phaseshift has been considered in detail (Lin 1975b; H. Klar and Fano 1976; H. Klar 1977; H. Klar and M. Klar 1978). Meanwhile recent experimental data of Wuilleumier *et al.* (1980) and Woodruff and Samson (1980) on the photoionization cross section of He with excitation of the ion to the $n = 2$ state are much lower just above threshold than predicted by close-coupling calculations (Jacobs and Burke 1972; Hyman *et al.* 1972), thereby indicating a need to improve the description of the two-electron correlations involved. Motivated by this discrepancy between theory and experiment, we have begun the investigation of the photoionization of He using the hyperspherical coordinate method. We report here our first results: adiabatic approximation calculations of the photoionization cross section for the process $\text{He} + \gamma \rightarrow \text{He}^+(1s) + e^-$. Our single-channel results, which lie 1% above the recently revised experimental data of Samson (1976) at threshold, 4% below at 1 Ryd above

threshold, and 12% below at 1.9 Ryd above threshold, compare well with the more detailed RPA (Wendin 1970; Amusia *et al.* 1974), close-coupling (Burke and McVicar 1965; Jacobs 1971), and polarized orbital (Bell and Kingston 1967) calculations, particularly at threshold.

In the hyperspherical coordinate method of Macek (1968), a two electron wavefunction $\psi(r_1, r_2)$ is expanded in terms of a complete set of adiabatic eigenfunctions $\varphi_\mu(R, \alpha, \hat{r}_1, \hat{r}_2)$, which depend parametrically on the hyperspherical radius $R \equiv (r_1^2 + r_2^2)^{1/2}$ and are functions of the five angular variables $\alpha \equiv \tan^{-1}(r_2/r_1)$, \hat{r}_1 , and \hat{r}_2 . The form of ψ is thus

$$\psi(R, \alpha, \hat{r}_1, \hat{r}_2) = (R^{5/2} \sin \alpha \cos \alpha)^{-1} \sum_{\mu} F_{\mu}(R) \varphi_{\mu}(R, \alpha, \hat{r}_1, \hat{r}_2) \quad (1)$$

The angular function φ is defined to satisfy the following differential equation in atomic units ($\hbar = e = m = 1$):

$$\frac{d^2}{d\alpha^2} - \frac{L_1^2}{\cos^2 \alpha} - \frac{L_2^2}{\sin^2 \alpha} + 2R \left(\frac{Z}{\cos \alpha} + \frac{Z}{\sin \alpha} - (1 - \sin 2\alpha \cos \theta_{12})^{-1/2} \right) \varphi_{\mu} = U_{\mu}(R) \varphi_{\mu}. \quad (2)$$

Here L_i^2 is the squared orbital angular momentum operator for the i th electron, $\theta_{12} \equiv \cos^{-1} \hat{r}_1 \cdot \hat{r}_2$, Z is the nuclear charge and $U_{\mu}(R)$ is the eigenvalue, which is parametrically dependent on R . Upon substituting equation (1) in the two-electron Schrödinger equation and using equation (2), one obtains the following set of coupled differential equations for the radial functions $F_{\mu}(R)$:

$$\begin{aligned} \frac{d^2}{dR^2} + \left[\frac{U_{\mu}(R) + \frac{1}{4}}{R^2} + \left(\phi_{\mu}, \frac{\partial^2 \phi_{\mu}}{\partial R^2} \right) + 2E \right] F_{\mu}(R) \\ + \sum_{\mu' \neq \mu} \left[\left(\phi_{\mu}, \frac{\partial^2 \phi_{\mu'}}{\partial R^2} \right) + 2 \left(\phi_{\mu}, \frac{\partial \phi_{\mu'}}{\partial R} \right) \frac{\partial}{\partial R} \right] F_{\mu'}(R) = 0. \end{aligned} \quad (3)$$

In equation (3) the coupling matrix elements $(\varphi_{\mu}, \partial^n \varphi_{\mu'} / \partial R^n)$, $n = 1, 2$, involve integration over the five angular variables only and are thus parametrically dependent on R . Given initial- and final-state wavefunctions ψ_i and ψ_f in the form of equation (1), the dipole amplitude for incident radiation linearly polarised along the z axis is

$$\langle \psi_i | \sum_{i=1}^2 \hat{\mathbf{e}} \cdot \mathbf{r}_i | \psi_f \rangle = \sum_{\mu\mu'} \int_0^{\infty} dR F_{\mu'}^i(R) R F_{\mu}^f(R) I_{\mu'\mu}(R) \quad (4a)$$

where

$$\begin{aligned} I_{\mu'\mu}(R) = \int d\alpha \int d\hat{r}_1 \int d\hat{r}_2 [\phi_{\mu'}^i(R, \alpha, \hat{r}_1, \hat{r}_2) \\ \times (\cos \alpha \cos \theta_1 + \sin \alpha \cos \theta_2) \phi_{\mu}^f(R, \alpha, \hat{r}_1, \hat{r}_2)]. \end{aligned} \quad (4b)$$

In calculating our wavefunctions we make an adiabatic approximation in which we keep only a single term μ in the summation in equation (1). For the ground state this term corresponds to the dominant $1s^2(^1S)$ configuration; for the final state this term corresponds to the dominant $1s\epsilon p(^1P)$ configuration. However, this adiabatic approximation is *not* an independent particle approximation; much correlation is included. (For example, in calculating φ_{μ}^i for the initial state, using equation (2), an expansion is made in the angular momentum pairs ss , pp , dd , and ff ; in calculating φ_{μ}^f for the final state, an expansion is made in the angular momentum pairs sp , ps , pd , dp , df , and fd .) In Table 1, we compare the He

Table 1. Non-relativistic total energies for the ground state of helium.

Source	Energy (au) ^a
Hartree-Fock ^b	-2.861 68
Present results: adiabatic upper bound	-2.895 17
Pekeris (1958)	-2.903 72
Present results: adiabatic lower bound	-2.929 67

^a 1 au = 27.2108 eV.

^b Clementi and Roetti (1974).

non-relativistic ground-state energy calculated in two hyperspherical adiabatic approximations with the essentially exact result of Pekeris (1958) as well as the Hartree-Fock (HF) result (Clementi and Roetti 1974). One adiabatic approximation includes the diagonal coupling matrix element ($\varphi_{\mu'}, \partial^2 \varphi_{\mu'} / R^2$) in solving equation (3), and the other ignores this term. In the former (resp. latter) case the lowest energy of each symmetry obtained upon solving equation (3)—ignoring all off-diagonal coupling terms—may be shown to give an upper (resp. lower) bound on the true energy (see *e.g.* Starace and Webster 1979). Our two adiabatic results do indeed bound the Pekeris result and are much more accurate than the HF result. In our photoionization calculations, both initial and final radial wavefunctions were calculated with the diagonal coupling term included. Indeed, this term is needed in order that equation (3) for $F_{\mu}(R)$ has the proper asymptotic form to $O(R^{-2})$ (Macek 1968).

The photoionization cross section obtained using only the lowest $\mu = 0$ term in equation (1) for the ¹S initial- and ¹P final-state wavefunctions is shown in Figure 1. Figure 1 also shows the revised experimental data of Samson (1976), which

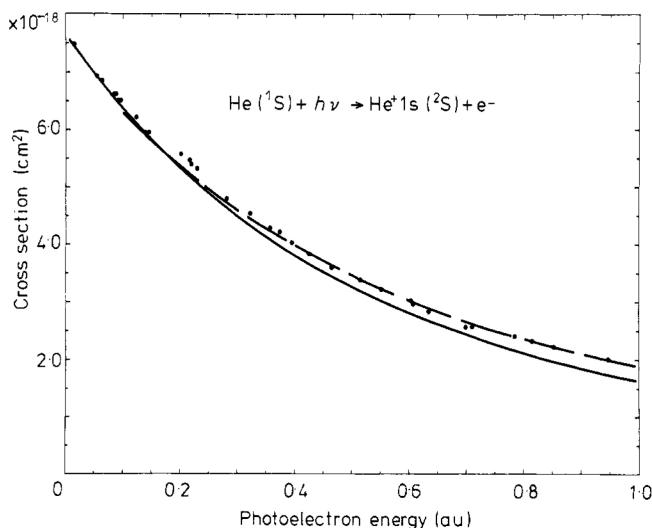


Figure 1. Photoionization cross section for He. Full curve, present adiabatic calculations in the hyperspherical coordinate method; broken curve, 1s-2s-2p close-coupling calculation of Jacobs (1971); dots, experimental measurements of Samson (1976).

Table 2. Comparison of the present results with some of the more detailed theoretical calculations of the photoionization cross section for the process $\text{He} + \gamma + \text{He}^+(1s) + e^-$.

Photo-electron energy (au) ^a	σ (Mb) ^b				
	Interpolated experimental results (Samson 1976) ^c	Hyperspherical coordinate method (present adiabatic results) ^d	RPA method (Wendin 1970,1971) ^e	Close -coupling method (Jacobs 1971) ^f	Polarized orbital method (Bell and Kingston 1967) ^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 au = 27.2108 eV.

^b Theoretical results are given in dipole length approximation. When available, dipole velocity results are given in parentheses.

^c Linear interpolation of the densely spaced experimental results (see Figure 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 Numerical values were supplied to us by Wendin.

^f See Table 4. Final state is obtained from a $1s-2s-2\bar{p}$ expansion. Initial state is the 56-term Pekeris variational wavefunction.

^g See table 2. Initial state is the 20-term Hart-Herzberg variational wavefunction.

have error bars of $\pm 3\%$. Our results lie within these error limits near threshold (for kinetic energies $0.0 \leq \epsilon \leq 0.4$ au) but are lower than experiment at higher energies. Of the many other theoretical calculations, we show the one with the best overall agreement with experiment: the three-channel (*i.e.* $1s-2s-2\bar{p}$) close-coupling calculations of Jacobs (1971). Our single-channel calculations do not include coupling to excited states of He^+ .

More quantitative comparison of our results with some other detailed theoretical calculations is shown in table 2. Within the kinetic energy range $0.0 \leq \epsilon \leq 0.25$ au, our values are comparable to those of these other calculations. Above $\epsilon = 0.25$ au the RPA (Wendin 1971) and polarized orbital (Bell and Kingston 1967) calculations lie higher than experiment, while our results lie lower. Close-coupling results (Jacobs 1971) are not given below $\epsilon = 0.1$ because of numerical problems near threshold; above $\epsilon = 0.25$ au they are in best agreement with experiment.

We are presently investigating the effect of higher final-state adiabatic channels, in particular those corresponding to $n = 2$ and $n = 3$ excitations. The need to include such higher channels is indicated by the adiabatic phaseshifts. At threshold our calculated phase for the $1s\epsilon p(^1P)$ channel is -0.151 rad. This compares with an extrapolated experimental value (Seaton 1966) of -0.041 rad. In contrast the $1s6p(^1P)$ energy level calculated (M. Klar 1977) *without* the diagonal coupling matrix element corresponds to a quantum defect of $+0.056$, which implies a threshold phaseshift of $+0.176$ rad. Thus, since omission or inclusion of the diag-

onal coupling matrix element in the adiabatic hyperspherical coordinate method can change the threshold phaseshift by 0.3 rad, it is quite likely that inclusion of off-diagonal coupling matrix elements in solving equation (3) will improve our calculated phaseshifts.

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