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Multiconfiguration Hartree-Fock calculation for the bound-free photodetachment cross section of H$^-$

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The photodetachment cross section of the H$^-$ ion has been obtained with the multiconfiguration Hartree-Fock method extended to compute the multiconfiguration Hartree-Fock continuum wave function. The electron correlation and polarization effects that are very important for photodetachment cross-section calculation have been taken into account in an *ab initio* manner through the configuration-interaction procedure. Our results are compared with other accurate and elaborate theoretical calculations and with experiment. It is found that the present results are in excellent agreement with experiment throughout the range of energies considered. The theoretical results obtained by other accurate methods are also in very close agreement with the present results.

I. INTRODUCTION

The theoretical study of electron correlation and polarization effects is presently one of the important lines of research in photoionization of atoms and ions. Negative ions are ideal candidates in this context. They are characterized by short-range electron correlation effects of the outer-shell electrons and long-range polarization of the core due to the continuum electron.

The photodetachment of negative ions is one of the important processes in determining the opacity of the solar atmosphere. In particular, the solar emissivity is controlled by H$^-$, through bound-free and free-free transitions. A large number of theoretical investigations have been carried out in the bound-free transitions of this system due to the fact that it is a simple, but nontrivial, theoretical exercise leading to clear interpretation of various theoretical approximations and methods. The photodetachment cross section of H$^-$ has been calculated by, among many others, Chandrasekhar,[1] Geltman,[2] Doughty *et al.*,[3] Bell and Kingston,[4] Ajmera and Chung,[5] Broad and Reinhardt,[6] Langhoff *et al.*,[7] Stewart,[8] Wishart,[9] Daskhan and Ghosh,[10] and most recently by Park *et al.*,[11] and Fink and Zoller.[12] Their main effort has been made to use increasingly more accurate wave functions for both the bound and the free states. Geltman[2] has evaluated the cross section using the 70-parameter bound-state wave function of Schwartz[13] together with a variationally determined symmetrized continuum function containing terms corresponding to the excited states of the hydrogen atom. Doughty *et al.*[3] have calculated the absorption cross section with the same 70-parameter Schwartz bound-state and a six-state close-coupling continuum function obtained by Hartree-Fock eigenfunction expansion. Bell and Kingston[4] have used the Schwartz bound-state function and a polarized orbital continuum function to determine the absorption cross section. Ajmera and Chung[5] used a bound-state wave function due to Rotenberg and Stein[14] who used the Hylleraas[15] correlated wave function with a tail function added to it. Their free-state wave function was calculated using the simplified Kohn-Feshbach variational method.[16] Broad and Reinhardt[6] used the elaborate multichannel *J*-matrix technique to solve the pseudostate close-coupling equations in order to obtain correlated wave functions for both the bound and the free state. Langhoff *et al.*[7] computed photoabsorption cross section of H$^-$ using Stieltjes and Tchebycheff moment techniques[17] from input generated from a configuration interaction calculation using square integrable basis functions. Stewart[8] used a perturbation-variation method to calculate the cross section, giving special consideration to the asymptotic part of the H$^-$ bound-state wave function. Wishart[9] obtained both the bound- and the free-state wave function using the close-coupling expansion method with the addition of the Hylleraas-type correlation terms. Daskhan and Ghosh[10] used a polarized orbital method to calculate the photodetachment cross section. They included the effect of distorted target wave function that has been neglected by Bell and Kingston.[4] Very recently Park *et al.*[11] and Fink and Zoller[12] used an adiabatic hyperspherical approximation to calculate the photodetachment cross section of H$^-$.

A comparison with the experimental results of Smith and Burch[18] still shows a significant difference between the existing theoretical calculations and the experiment, especially for larger wavelengths.

It is found that the multiconfiguration Hartree-Fock (MCHF) approach has achieved considerable success in the calculation of the photoionization cross section of atoms. The first application of the MCHF method extended to compute continuum wave functions to photoionization processes was in the calculation of the photoionization of sodium atoms.[19,20] It achieved better agreement with experiment. From the point of view of photoabsorption, the MCHF approach is appealing because it takes into account electron correlation and polarization effects very efficiently. To determine the applicability of the MCHF method to the photodetachment of negative ions, we have undertaken an extensive calculation for the photodetachment cross section of H^-.

We performed this calculation for two reasons. We want to see how successfully the MCHF method can be applied to the calculation of the photodetachment cross section of negative ions by taking into account the correlation and polarization effects in *ab initio* manner through the configuration-interaction procedure.

II. THEORY

Recently Saha *et al.*[19,20] applied the MCHF method extended to compute the MCHF continuum wave function to study electron correlation and polarization effects in atomic photoionization. It is found that the MCHF method can take into account the short-range correlation and the long-range polarization effects very accurately. In their method of calculation, an MCHF wave function for a continuum state could be expressed in terms of correlated ionic core with an outer continuum electron and other bound-state contributors. In the calculation of the photodetachment of negative ions, the MCHF code is further extended to calculate the final free-state wave functions. These wave functions are found to be very accurate at all electron separations.

A. The MCHF theory of photodetachment

The photodetachment cross section is given by

$$\sigma_L = \frac{4\pi^2 \alpha a_0^2 \omega}{3} \sum_f \left| \left\langle \Psi_f \left| \sum_{j=1}^{n} z_j \right| \Psi_i \right\rangle \right|^2 , \tag{1}$$

$$\sigma_V = \frac{4\pi^2 \alpha a_0^2 \omega}{3} \sum_f \left| \left\langle \Psi_f \left| \sum_{j=1}^{n} \frac{\nabla_j^z}{i\omega} \right| \Psi_i \right\rangle \right|^2 . \tag{2}$$

Equations (1) and (2) represent, respectively, the length and the velocity formulas. The wave functions Ψ_i and Ψ_f represent, respectively, the bound and the free states of the negative hydrogen ion. ω is the photon energy in atomic units. α and a_0 are, respectively, the fine-structure constant and Bohr radius of the hydrogen atom. The sum runs over all final-state configurations. The length and the velocity forms of the cross sections will give identical results if the bound- and the free-state wave functions are exact.

B. The MCHF wave function for the final continuum state

The final state is a neutral hydrogen atom and a free electron. The MCHF wave function for the final free state with label γ, energy E, and term LS is expanded in a series of the form

$$\Psi(\gamma LS; N+1) = \sum_{j=1}^{m_c} a_j \Phi(\gamma_j L_c S_c; N)\phi_{kl} + \sum_{i=1}^{m} c_i \Phi(\gamma_i LS; N+1) , \tag{3}$$

where the first term describes an N-electron core that is an eigenstate of L_c and S_c, in terms of N-electron bound configuration states $\Phi(\gamma_j L_c S_c; N)$ with configuration γ_j and term $L_c S_c$, mixing coefficients a_j and total energy E_c coupled with a continuum orbital ϕ_{kl} of angular momentum l to yield an antisymmetric configuration state for the $(N+1)$-electron bound-state configurations which are eigenstates with the same L and S and which are included to allow for electron correlation and the core polarization.

A set of radial functions, say, $P_i(r)$, $i=1,\ldots,m$ defines the above MCHF wave function. All the radial functions are solutions of the coupled integro-differential equations of the form

$$\left[\frac{d^2}{dr^2} + \frac{2z}{r} - \frac{l(l+1)}{r^2} \right] P_i(r) = \frac{2}{r}[Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{i'} \varepsilon_{ii'} P_{i'}(r) . \tag{4}$$

The off-diagonal energy parameters $\varepsilon_{ii'}$ are related to Lagrange multipliers to ensure orthogonality assumptions. (For an explanation of the terms in the equation, see Ref. 19.) In the MCHF method for the free state, all the radial functions describing the core are assumed to be fixed along with the mixing coefficients a_j. Other bound-state radial functions are determined variationally along with the radial function for the continuum electron.

The boundary condition satisfied by the bound radial functions are

$$P_i(r) \underset{r\to 0}{\sim} r^{l+1}, \quad P_i(r) \underset{r\to\infty}{\sim} 0 .$$

In this case the diagonal energy parameter ε_{ii} is an eigenvalue of the integro-differential equation and hence needs to be determined. The radial functions for the continuum orbital satisfy the following boundary conditions:

$$\begin{aligned} P_i(r) &\underset{r\to 0}{\sim} r^{l+1} , \\ P_i(r) &\underset{r\to\infty}{\sim} k^{-1/2} \sin\left[kr - \frac{l}{2}\pi + \eta_l \right] , \end{aligned} \tag{5}$$

where η_l is the phase shift and $\varepsilon_{ii} = -k^2$, k^2 being the kinetic energy of the continuum electron.

The coupled integro-differential equations are solved numerically by the iterative method. The multiconfiguration (MC) self-consistent field (SCF) procedure is applied to compute both the bound and the continuum wave functions. The same numerical procedures are used for both the bound and the continuum wave functions. The bound radial functions are essentially bound in nature and vary smoothly as $r \to \infty$. The continuum radial function is normalized by fitting the computed values at two adjacent points to the regular and irregular Bessel functions as soon as the region where the direct and the exchange potentials are vanishingly small is reached, which may be considerably smaller values of r than the asymptotic form represented by the boundary condition of Eq. (5).

The coefficients c_i, which need to be determined, are solutions of the system of equations derived from the condition that $\langle \Psi | H - E | \Psi \rangle$ is stationary with respect to the variations in the coefficients, where H is the Hamiltonian for the $(N+1)$-electron system and $E = E_c + k^2/2$ (in atomic units).

The coefficients c_i are solutions of the system of equations

$$\sum_{i'=1}^{m} \langle \Phi_i \mid H-E \mid \Phi_{i'} \rangle c_{i'} + \sum_{j=1}^{m_c} \langle \Phi_i \mid H-E \mid \Phi_j \rangle a_j = 0 \, , \qquad i=1,\ldots,m$$

where

$$\Phi_j \equiv \Phi(\gamma_j L_c S_c ; N) \cdot \phi_{kl}, \quad j=1,\ldots,m_c$$

and

$$\Phi_i \equiv \Phi(\gamma_i LS : N+1), \quad i=1,\ldots,m \, .$$

III. COMPUTATIONAL PROCEDURE

In order to take into account the electron correlation and the core polarization very accurately, a large number of configurations were selected. The MCHF method described in the previous papers[19-21] has been used to perform the present calculations. Briefly, the MCHF method[22] for the bound state is used to determine a set of bound radial functions. The modified MCHF method[21] for the continuum wave functions was applied to determine a set of bound and continuum wave functions for a range of kinetic energy of the continuum electron.

A. Initial bound-state wave function: $1s^2\,{}^1S$

The initial state is the ground state of the H^- ion. The MCHF wave-function expansion for the initial state of the H^- ion was over the set of 32 configuration states, coupled to form a ${}^1\mathrm{S}$ term:

$$\{ 1s^{2,} 1s2s, 2s^2, 2p^2, 1s3s, 2s3s, 2p3p, 3s^2, 3p^2, 3d^2, 1s4s, 2s4s, 2p4p, 3s4s, 3p4p, 3d4d, 4s^2, 4p^2$$
$$4d^2, 4f^2, 1s5s, 2s5s, 2p5p, 3s5s, 3p5p, 3d5d, 4s5s, 4p5p, 4d5d, 5s^2, 5p^2, 5d^2 \} \; {}^1S \, .$$

The above set of configurations was selected in the expansion, so that its contribution toward the dipole matrix element is appreciable. The radial wave functions for the different orbitals were obtained by the MCHF procedure, varying all the orbitals simultaneously except 1*s*, which was obtained from the Hartree-Fock (HF) calculation of the hydrogen atom and was kept fixed. Minimization of the total energy yielded an energy of −0.527 542 1 a.u., to be compared to an accurate value of −0.527 750 9 a.u from the extensive Pekeris calculation.[23]

B. Final-state wave function: $1skp\ {}^1P^0$

The final-state continuum wave function expansion for the singlet *P* state of H^- contains 36 configurations:

$$\{ 1skp, 1s2p, 2s2p, 2p3s, 2p3d, 2p4s, 2p4d, 2p5s, 2p5d, 1s3p, 1s4p, 1s5p, 2s3p, 2s4p, 2s5p, 3s3p \, ,$$
$$3s4p, 3s5p, 3p3d, 3p4s, 3p4d, 3p5s, 3p5d, 3d4p, 3d4f, 3d5p, 4s4p, 4s5p, 4p4d, 4p5s \, ,$$
$$4p5d, 4d4f, 4d5p, 4f5d, 5s5p, 5p5d \} \; {}^1P^0 \, .$$

The radial function 1*s* was kept fixed to the Hartree-Fock 1*s* of a hydrogen atom. The final-state radial functions were obtained by varying all other orbitals including *kp* simultaneously. The above set of configurations was selected after a series of tests had been performed, and represents the set of configurations which contributes considerably to the dipole matrix elements.

IV. EVALUATION OF RESULTS

Using the wave function for the initial bound state and the final continuum state the dipole matrix elements in the length and velocity forms were calculated to obtain the photodetachment cross section of H^-. We obtained the electron affinity of H as 0.027 542 1 a.u., which is very close to the accurate value 0.027 750 9 a.u. We used this calculated energy for the photodetachment cross-section calculation.

We presented in Table I, the results for the cross section calculated using the MCHF approach for the initial ground state consisting of 32 configurations and the modified MCHF method for the final free state containing 36 configurations. The present length and velocity cross sections are in excellent agreement for k^2 ranging from 0.0025 to 0.70 Ry, which indicates that our wave-function expansions for the initial and the final states are very accurate. The results from the previous calculations by Bell and Kingston,[4] Ajmera and Chung,[5] Broad and Reinhardt,[6] Stewart,[7] Wishart,[8] and Daskhan and Ghosh[9] are included in the table for comparison. Daskhan and Ghosh[9] and Wishart[8] made calculations for the length cross sections only, so comparison is not possible with the present velocity results. Daskhan and Ghosh (DG) used the polarized orbital method to calculate the photodetachment cross section of H^-. They considered the dipole matrix element involving the distorted target wave function that had been neglected by Bell and Kingston. A comparison of present length results with the result of DG shows that for $k^2 < 0.04$ and for $k^2 \geq 0.08$, their results are lower than ours. For $0.04 \leq k^2 \leq 0.08$, their results are a little higher. It should be remembered that polarized orbital method takes into account the long-range polarization but neglects the short-range correlation. Wishart obtained

TABLE I. Comparison of present photodetachment cross section of H^- (in units of 10^{-17} cm^2) as a function of photoelectron energy (Ry) with other theoretical calculations.

k^2	Present		DG[a]	W[b]	S[c]		BR[d]		AC[e]		BK[f]	
(Ry)	L	V	L	L	L	V	L	V	L	V	L	V
0.0025	0.284	0.279									0.190	0.281
0.005	0.709	0.698									0.502	0.712
0.01	1.554	1.52	1.221	1.553	1.565	1.566			1.531	1.408	1.234	1.625
0.02	2.868	2.846	2.559	2.846	2.862	2.870	2.798	2.852	2.810	2.668	2.600	3.070
0.03	3.583	3.568	3.461		3.580	3.595			3.525	3.406	3.540	3.903
0.04	3.911	3.891	3.920	3.898	3.912	3.935	3.982	3.885	3.863	3.718	4.048	4.295
0.05	4.007	3.990	4.100		4.010	4.040			3.968	3.856	4.231	4.414
0.06	3.968	3.957	4.080	3.965	3.978	4.012	3.956	3.891	3.940	3.860	4.205	4.375
0.07	3.857	3.847	3.950		3.870	3.910			3.838	3.760	4.060	4.254
0.08	3.707	3.695	3.663	3.708	3.717	3.757	3.759	3.759	3.695	3.642	3.859	4.090
0.09	3.538	3.529	3.409		3.548	3.589			3.533	3.500	3.640	3.910
0.10	3.364	3.360		3.368	3.373	3.414	3.313	3.331	3.364	3.351	3.432	3.733
0.117	3.074	3.072		3.078	3.068	3.109	3.019	3.024	3.06	3.01	3.08	
0.16	2.443	2.443	2.335		2.45	2.48	2.41	2.40	2.463	2.481	2.447	3.753
0.25	1.599	1.600	1.541		1.595	1.611	1.591	1.588			1.643	1.818
0.36	1.065	1.068	1.064		1.058	1.061	1.072	1.063	1.094	1.145	1.129	1.194
0.50	0.722	0.724		0.728	0.716	0.712	0.729	0.718				
0.64	0.553	0.555	0.523		0.547	0.542	0.560	0.577	0.584	0.626	0.531	0.548
0.70	0.525	0.530		0.539	0.523	0.518	0.543	0.542				

[a] DG, Daskhan and Ghosh (Ref. 10).
[b] W, Wishart (Ref. 9).
[c] S, Stewart (Ref. 8).
[d] BR, Broad and Reinhardt (Ref. 6).
[e] AC, Ajmera and Chung (Ref. 5).
[f] BK, Bell and Kingston (Ref. 4).

accurate bound- and free-state wave functions using a close-coupling pseudostate expansion with the addition of Hylleraas-type correlation terms. Their length results are in excellent agreement with the present length results. Ajmera and Chung used a 33-parameter Hylleraas-type ground-state wave function with a "tail function" included to achieve the correct asymptotic form. This free-state wave function was calculated using the simplified Kohn-Feshbach variational method. Their length results are very close to the present length results. For $k^2 < 0.117$, their results are a little lower, and for $k^2 \geq 0.117$, their results are slightly higher. Their velocity results are lower than the present velocity results for $k^2 < 0.117$, and are higher for $k^2 > 0.117$. Stewart used a perturbation-variation method, giving special attention to the asymptotic part of bound-state wave function. At low energies the present length results agree very well with those of Stewart. At high energies their results are a little lower. Compared to Stewart's velocity results, the present velocity results are a little lower at low energies but higher at high energies. Broad and Reinhardt used the multichannel J-matrix technique to solve the pseudostate close-coupling equations using only L^2 basis functions. They used a set of 67 ^1S two-electron configurations constructed from $8s$, $6p$, and $4d$ one-electron Slater orbitals for the ground state. For the continuum, they used basis sets constructed from $10s$, $10p$, and $6d$ orbitals giving 160 configurations and 36 approximate scattering channels. Their results are in close agreement with the present results. Bell and Kingston (BK) used the polarized orbital method to represent the symmetrized continuum function. A comparison with the best length results of BK shows that for $k^2 < 0.04$, their cross section is lower than the present length cross section but for $0.04 \leq k^2 \leq 0.36$, their results are higher. Their velocity results are higher than their length results. Since the polarized orbital method takes into account the long-range polarization but neglects short-range correlation, according to BK, their length calculation can be expected to be more accurate than their velocity results. The close agreement between our length and velocity results and excellent agreement between the present results and the accurate results of Wishart[8] and Stewart[7] reveals that the present length and velocity cross sections are better.

In Fig. 1 we plotted the present length and velocity cross sections as a function of incident photon wavelength from 4000 to 15 000 Å. The relative experimental cross sections measured by Smith and Burch,[18] normalized to the present length curve at 5280 Å ($k^2 = 0.117$ Ry) have been included in the figure for comparison. These experimental measurements have an estimated uncertainty of less than 3% and have been put on an absolute basis by Geltman[2] from the absolute integrated measurements of Branscomb and Smith,[24] with the value of 3.28×10^{-17} cm^2 at 5280 Å within an uncertainty of about 10%. Our values of the cross section at 5280 Å are 3.074×10^{-17} cm^2 in the length form and 3.072×10^{-17} cm^2 in the velocity form and are in excellent agreement with the value 3.28×10^{-17} cm^2 $\pm 10\%$ obtained from ab-

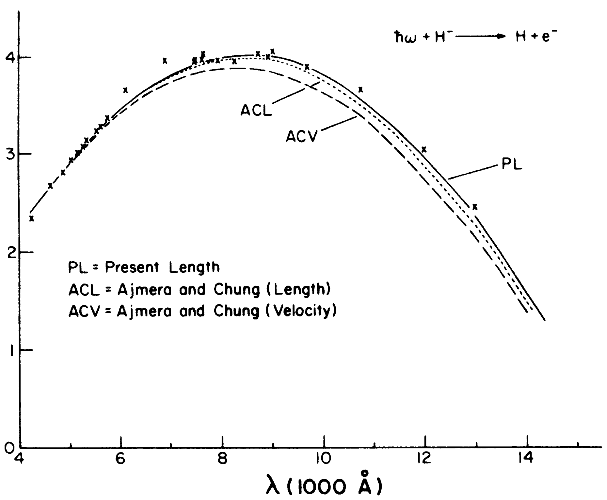

FIG. 1. Photodetachment cross section of H^- vs photon wavelength. ×, experimental results of Smith and Burch; ——, present correlated length (PL); — — —, Ajmera and Chung length (ACL); ———, Ajmera and Chung velocity (ACV) results.

solute measurement. These results may be compared with 3.08×10^{-17} cm^2 (length) of Wishart, 3.07×10^{-17} cm^2 (length), and 3.11×10^{-17} cm^2 (velocity) of Stewart; 3.02×10^{-17} cm^2 (length and velocity) of Broad and Reinhardt, 3.06×10^{-17} cm^2 (length), and 3.01×10^{-17} cm^2 (velocity) of Ajmera and Chung, 3.01×10^{-17} cm^2 of Kim[25] from the moment adjusted method, 2.96×10^{-17} cm^2 of Doughty *et al.*, and 2.99×10^{-17} cm^2 of Geltman. As the present length and velocity results are very close, we could not show the difference in the figure. We also plotted the length and velocity results of Ajmera and Chung for comparison. Our length and velocity results agree very well with experiment throughout the range of wavelength considered. More specifically, our result is in better agreement in the large wavelength region compared to other theoretical results. It should be mentioned here that very recently Park *et al.*[11] computed photodetachment cross section of H^- using the adiabatic hyperspherical approximation. Near the peak in the cross section at 0.03 a.u. above threshold their length results are 12% higher than the length results of Stewart. At high energies near 0.275 a.u. their results are about 20% lower than the length results of Stewart. Fink and Zollar[12] used the same adiabatic hyperspherical approximation to calculate the photodetachment cross section of H^-. The maximum of their cross section is overestimated, while their cross section becomes too small with increasing energy. Compared with Park *et al.*, their results agree within 1%.

V. CONCLUSION

Extensive studies of the photodetachment cross section of H^- over a range of photon wavelengths, 4000–15 000 Å, have been performed using the multiconfiguration Hartree-Fock approximation. Short-range correlation and long-range dynamical polarization effects that are very important for the photodetachment cross section of negative ions have been taken into account adequately and in an *ab initio* manner through the configuration-interaction procedure. In comparing the theoretical results with experiment it is found that the present results predict cross section very accurately throughout the range of wavelengths considered. The present results are in excellent agreement with the accurate calculation of Wishart[8] and Stewart[8] and also with other theoretical calculations by Ajmera and Chung,[5] Broad and Reinhardt,[6] and Langhoff *et al.*,[7] who used elaborate methods in calculating the photodetachment cross section of negative hydrogen ions. Because Wishart calculated only the length form of the cross section, it is not possible to compare the present velocity results with his calculation. The polarized orbital method used by Daskhan and Ghosh and Bell and Kingston does not take into account the short-range correlation. Moreover, this method cannot consider the long-range polarization in an *ab initio* way. Excellent agreement between the present length and velocity cross sections shows the accuracy of the initial- and final-state wave functions. Finally we conclude that MCHF method modified for continuum wave function, which is general and can take into account the correlation and polarization effects very accurately and in an *ab initio* manner in comparison to other elaborate theoretical methods, predicts reliable results.

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