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Photodetachment cross section of the negative hydrogen ion

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The photodetachment cross section of the H⁻ ion has been obtained with the use of two variants of the polarized-orbital method. Calculation takes into account the matrix elements involving a distorted-target wave function that has been neglected by Bell and Kingston. The results have been compared with other theoretical results.

I. INTRODUCTION

We consider the bound-free absorption coefficients of the H⁻ ion. In the past, efforts have been made to employ increasingly more accurate wave functions for both the bound and the free states. Geltman,[1] Doughty *et al.*,[2] and Bell and Kingston[3] have used the 70-parameter bound-state wave functions of Schwartz (unpublished) to include the correlation effect properly. The continuum-state wave functions as used by them have included the effect of the inelastic channels. However, the method of inclusion of this effect is different.

Recently, Stewart[4] and Wishart[5] have calculated the cross section for photodetachment in the H⁻. Stewart employed a perturbation-variation method to calculate the cross section. Wishart obtained both the bound and the free state using the close-coupling expansion method with the addition of the Hylleraas-type correlation terms.

Here we have extended the work of Bell and Kingston (BK) in which the symmetrized continuum function is represented by a polarized-orbital one. In their calculation they have neglected the matrix elements containing the distorted-target wave function. It is now believed that these matrix elements are important (Bhatia and Temkin,[6] McDowell and his co-workers,[7] in predicting the scattering parameters. Moreover, there are different variants of the polarized-orbital method (POM). BK have used the variant as prescribed by Temkin and Lamkin[8] (*p*-wave corrections are made by Sloan[9]).

Our motivation in this paper is twofold: We would like to see the effect of the matrix elements involving the distorted-target state and the effect of different variants of the POM. We have included the matrix elements involving the target-distortion wave function. Moreover, two variants of the POM have been used in calculating the bound-free absorption coefficients of the negative hydrogen ion. In addition to the commonly used method of Temkin, Lamkin, and Sloan, the variant of Daskhan *et al.*[10] has also been employed. It may be mentioned that POM, due to Temkin and Lamkin, includes the effect of the adiabatic dipole potential only. The variant of Daskhan *et al.* has its origin from the works of Callaway *et al.*[11] Their variant contains the adiabatic potential ($l = 0,1,2$) and a correction term to the adiabatic potential ($l = 0,1$). Two variants have been used to find its relative importance in predicting the absorption coefficients.

II. THEORY

It is well known that the POM fails to incorporate the short-range correlations. It takes into account the long-range polarization effect properly. Therefore, the free-state wave function obtained by using the POM is believed to be inaccurate at small and intermediate electron separations. The velocity formulation is sensitive to the accuracy of the free-state wave function at small and intermediate electron separations. On the other hand, the length formulation weighs on the large electron separation region. Therefore, the length-formulation results are believed to be reliable when one uses the polarized-orbital free-state function. This has also been pointed out by BK. The photodetachment cross section or the absorption coefficient of the H⁻ in the length formulation is given by

$$K_L = 6.812 \times 10^{-20} k (k^2 + 2I) \left| \int \Psi_F^*(z_1 + z_2)\Psi_B d\tau \right|^2 \quad (1)$$

in units of cm². The wave functions Ψ_B and Ψ_F represent the bound and free states of the negative hydrogen ion. k is the wave number (in atomic units) of the ejected electron and I denotes the electron affinity of hydrogen (in atomic units). The matrix elements are also expressed in atomic units.

The wavelength of the incident radiation is given by (in Å)

$$\lambda = \frac{911.267}{k^2 + 2I} . \quad (2)$$

Both the bound and free states are singlets and the nonzero contribution to the matrix element comes from the *p*-wave part of the free-state wave function. The bound-state wave functions used are the 20-parameter function of Hart and Herzberg[12] and the 70-parameter function of Schwartz. We have employed two free-state wave functions to calculate the absorption coefficient of the H⁻.

A. Model *A*

The free-state wave function is determined by the method of Daskhan *et al.* in the framework of POM. The corresponding integro-differential equation is given by

$$\left[\frac{d^2}{dr^2}+k^2+v(r)-\frac{l(l+1)}{r^2}\right]u_l(r)$$

$$\pm 4z^3 e^{-zr}\left[(k^2+z^2)r\delta_{l0}\int_0^\infty e^{-zr_2}r_2 u_l(r_2)dr_2\right.$$

$$\left.-\frac{2}{2l+1}\left[r^{-l}\int_0^r e^{-zr_2}r_2^{l+1}u_l(r_2)dr_2+r^{l+1}\int_r^\infty e^{-zr_2}r_2^{-l}u_l(r_2)dr_2\right]\right]$$

$$=v_d u_l(r)\mp 4z\, e^{-zr}\frac{1}{3}\left[\delta_{l1}[-\tfrac{1}{2}z(z^2+k^2)r^3+(z^2-k^2)r^2]\int_r^\infty e^{-zr_2}r_2^{-l}u_l(r_2)dr_2\right.$$

$$+2(\tfrac{1}{2}zr^3+r^2)\left[\frac{l}{(2l-1)(2l+1)}r^{l-1}\int_r^\infty e^{-zr_2}r_2^{-l-1}u_l(r_2)dr_2\right.$$

$$\left.\left.+\frac{l+1}{(2l+1)(2l+3)}r^{l+1}\int_r^\infty e^{-zr_2}r_2^{-l-3}u_l(r_2)dr_2\right]\right]$$

$$\pm\tfrac{4}{3}z\delta_{l1}e^{-2zr}\left[(\tfrac{3}{2}z^2r^2+\tfrac{1}{2}zr-3)u_l(r_2)-(\tfrac{1}{2}zr^2+r)\frac{d}{dr}u_l(r)\right],\tag{3}$$

where V_d is the distortion potential and

$$V(r)=2(z-1)/r+2\left[z+\frac{1}{r}\right]e^{-2zr}.$$

The distortion potential consists of the sum of the first three multipole components ($l=0,1,2$) of the adiabatic polarization potentials plus the first two components ($l=0,1$) of the nonadiabatic distortion potential. The distortion potential is the same as Callaway et al.

B. Model B

The free-state wave function is due to Temkin, Lamkin, and Sloan. The corresponding integro-differential equation is obtained by replacing V_d by $\beta(zr)/(zr)^4$ in Eq. (3), where

$$\beta(x)=\tfrac{9}{2}-\tfrac{2}{3}e^{-2x}(x^5+\tfrac{9}{2}x^4+9x^3$$

$$+\tfrac{27}{2}x^2+\tfrac{27}{2}x+\tfrac{27}{4}).$$

III. RESULTS

In Table I we have tabulated our results for the absorption coefficients for the two symmetrized continuum-wave functions which have been obtained by solving the integro-differential equation (3). For the bound-state wave function we have used the 20-parameter wave function of Hart and Herzberg. Comparison of the present results (model B) with the corresponding results of BK suggests that the inclusion of the matrix elements involving the distorted-target function is important. This feature has also been noticed in other scattering calculations. The results of the model A which have been obtained by using the free-state function of Daskhan et al. are very close to those of model B. Similar behavior has also been noticed by Daskhan et al. in elastic e^--H scattering and by Basu et al.[13] in the corresponding excitation problem. The present results that have been obtained using the 70-parameter wave function of Schwartz are tabulated in

Table II. The results of other elaborate theoretical calculations have also been included for comparison. The four theoretical calculations by Stewart,[4] Wishart,[5] Broad and Reinhardt,[14] and Ajmera and Chung[15] are the most elaborate methods used in calculating the absorption coefficients of negative hydrogen; the calculations of Wishart and Stewart probably give the most accurate results. In the energy range considered the present results would be expected to be in better agreement with the earlier, more accurate, theoretical predictions than those of BK. Below the incident energy $k^2=0.04$, the results of the present calculations differ very little from those of BK. However, our results as well as those of BK, disagree with those of Wishart and Stewart. The effect of the matrix elements

TABLE I. Calculated absorption coefficients (in units of 10^{-17} cm^2) of the negative hydrogen ion in the length formulation using the 20-parameter bound-state function.

k^2 (a.u.)	λ (Å)	Model A present	Model B present	Bell and Kingston (Ref. 3)
0.0025	15 711	0.092	0.101	0.105
0.0075	14 464	0.561	0.490	0.501
0.0150	12 925	1.184	1.231	1.232
0.0200	12 069	1.807	1.675	1.719
0.0300	10 658	2.513	2.500	2.579
0.0350	10 069	2.780	2.838	2.931
0.0450	9067	3.397	3.345	3.469
0.0550	8247	3.748	3.672	3.805
0.0700	7261	3.784	3.822	4.013
0.0900	6263	3.772	3.702	3.933
0.1250	5049	3.102	3.108	3.382
0.1600	4229	2.477	2.470	2.762
0.2500	2983	1.483	1.470	1.662
0.3600	2193	0.925	0.903	1.067
0.6400	1310	0.535	0.505	0.542

TABLE II. Calculated absorption coefficients (in units of 10^{-17} cm^2) of the negative hydrogen ion in the length formulation.

k^2 (a.u.)	70-parameter model B		Stewart (Ref. 4)	Wishart (Ref. 5)	Broad and Reinhardt (Ref. 14)	Ajmera and Chung (Ref. 15)
	Bell and Kingston	Present				
0.01	1.234	1.221	1.57	1.553		1.531
0.02	2.60	2.559	2.86	2.846		2.81
0.03	3.54	3.461	3.58			3.52
0.04	4.05	3.920	3.91	3.898	3.98	3.86
0.05	4.231	4.100	4.01			3.97
0.06	4.210	4.080	3.98	3.965	3.96	3.94
0.07	4.06	3.950	3.87			3.84
0.08	3.86	3.663	3.72	3.708	3.76	3.70
0.09	3.640	3.409	3.55			3.53
0.16	2.447	2.335	2.45		2.41	2.46
0.25	1.643	1.541	1.595		1.591	
0.36	1.129	1.064	1.058		1.072	1.094
0.64	0.531	0.523	0.547		0.560	0.584

involving the target-distortion wave function is found to be appreciable for $k^2 \geq 0.04$. Our results in the energy range $0.04 \leq k^2 \leq 0.08$ are better than those of BK when one compares the results with those of Wishart and Stewart. Above these incident energies the present results have an accuracy similar to the results of BK. The present method, which is simple in comparison to other elaborate theoretical methods, predicts reliable results.

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[1]S. Geltman, Astrophys. J. 136, 935 (1962).

[2]N. A. Doughty, P. A. Fraser, and R. P. McEachran, Mon. Not. R. Astron. Soc. 132, 255 (1966).

[3]K. L. Bell and A. E. Kingston, Proc. Phys. Soc. London 90, 895 (1967).

[4]A. L. Stewart, J. Phys. B 11, 3851 (1978).

[5]A. W. Wishart, J. Phys. B 12, 3511 (1979).

[6]A. K. Bhatia and A. Temkin, Phys. Rev. A 12, 2044 (1975).

[7]T. Scott and M. R. C. McDowell, J. Phys. B 10, 1059 (1977).

[8]A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961).

[9]I. H. Sloan, Proc. R. Soc. London, Ser. A 281, 151 (1964).

[10]M. Daskhan, P. Khan, A. S. Ghosh, and Carlos Falcon, Phys. Rev. A 23, 728 (1981).

[11]J. Callaway, R. W. LaBahn, R. T. Pu, and M. M. Duxler, Phys. Rev. 168, 12 (1968).

[12]J. F. Hart and G. Herzberg, Phys. Rev. 106, 79 (1957).

[13]M. Basu, P. S. Majumdar, and A. S. Ghosh, Phys. Rev. A 26, 3000 (1982).

[14]J. T. Broad and W. P. Reinhardt, Phys. Rev. A 14, 2159 (1976).

[15]M. P. Ajmera and K. T. Chung, Phys. Rev. A 12, 475 (1976).