AIM

Association for Information and Image Management

1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202

Centimeter

Inches

MANUFACTURED TO AIM STANDARDS
BY APPLIED IMAGE, INC.

DYNAMICS OF COLLISION PROCESSES

Progress Report

for the Period September 1, 1991 – July 31, 1994

Anthony F. Starace

Department of Physics and Astronomy

The University of Nebraska

Lincoln, NE 68588-0111

N O T I C E

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product or process disclosed or represents that its use would not infringe privately-owned rights.

February 1994

Prepared for

THE U.S. DEPARTMENT OF ENERGY
AGREEMENT NO. DE-FG02-88ER13955

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

I. ABSTRACT

Investigations have been carried out of one-, two-, and three-photon detachment of the negative hydrogen ion (H^-) including effects of electron correlations, of two-color detachment of H^- with excitation of $H(n=2)$, and of the 3P_e state of H^- . Striking effects of long-range dipole field interactions have been demonstrated. Electron correlation effects on detachment cross sections have been quantified. Electric field effects on photodetachment of H^- above the $H(n=2)$ threshold have also been elucidated. Variational R-matrix calculations of photodetachment of H^- and of Li^- including excitations of the residual atoms up to the $n=6$ level have provided state-of-the-art agreement with recent experimental results. Furthermore, doubly-excited-state spectra of H^- and Li^- have been shown to be remarkably similar.

II. COMPLIANCE

Neither the aims of investigations nor the effort of the principal investigator to this project have deviated from what was proposed. During the present project period the principal investigator devoted 25% of his time to this project during 1 September 1991 – 31 December 1992. While on sabbatical at the Joint Institute for Laboratory Astrophysics at the University of Colorado–Boulder, he increased his effort to 50% of time during the period 1 January – 31 August 1992. Since 1 September 1992 his effort has returned to 25% of time.

III. BIBLIOGRAPHY

A. Articles

1. C.R. Liu, N.Y. Du, and A.F. Starace, ONE- AND TWO-PHOTON DETACHMENT OF H^- WITH EXCITATION OF $H(n=2)$, *Phys. Rev. A* **43**, 5891 (1991).
2. A.F. Starace, LONG-RANGE DIPOLE FIELD EFFECTS ON H^- DETACHMENT PROCESSES ABOVE THE $H(n=2)$ THRESHOLD, in *Atomic and Molecular Physics: Third US/Mexico Symposium, Morelos, Mexico, 13–16 March 1991*, edited by C. Cisneros, T.J. Morgan, and I. Alvarez (World Scientific, Singapore, 1991), pp. 359-378.
3. A.F. Starace, HYPERSPHERICAL COORDINATE DESCRIPTION OF SINGLE- AND MULTIPHOTON PROCESSES IN TWO-ELECTRON SYSTEMS, in *Many-Body Theory of Atomic Structure and Photoionization*, edited by Tu-Nan Chang (World Scientific, Singapore, 1993), pp. 107-142.
4. C.R. Liu, B. Gao, and A.F. Starace, VARIATIONALLY STABLE-TREATMENT OF TWO- AND THREE-PHOTON DETACHMENT OF H^- INCLUDING ELECTRON-CORRELATION EFFECTS, *Phys. Rev. A* **46**, 5985 (1992).
5. N.Y. Du, A.F. Starace, and N.A. Cherepkov, RESONANT TWO-COLOR DETACHMENT OF H^- WITH EXCITATION OF $H(n=2)$, *Phys. Rev. A* **48**, 2413 (1993).

6. N.Y. Du, I.I. Fabrikant, and A.F. Starace, ELECTRIC-FIELD EFFECTS ON H^- PHOTODETACHMENT WITH EXCITATION OF $H(n=2)$, Phys. Rev. A **48**, 2968 (1993).
7. C. Pan, A.F. Starace, and C.H. Greene, PARALLELS BETWEEN HIGH DOUBLY EXCITED STATE SPECTRA IN H^- AND Li^- PHOTODETACHMENT, J. Phys. B Lett. (Submitted).
8. N.Y. Du, A.F. Starace, and M.Q. Bao, PHOTODETACHMENT OF AND RADIATIVE ATTACHMENT TO THE $H^- 2p^2(^3P^e)$ STATE (to be submitted).

B. Conference Abstracts

9. N.Y. Du and A.F. Starace, RESONANT TWO-COLOR PHOTODETACHMENT OF H^- WITH EXCITATION OF $H(n=2)$, Bull. Am. Phys. Soc. **37**, 1141 (1992). [DOE Report No. DOE/ER/13955-14]
10. N.Y. Du, A.F. Starace, and M.Q. Bao, PHOTODETACHMENT OF THE $^3P^e$ STATE OF H^- , Bull. Am. Phys. Soc. **38**, 1124 (1993). [DOE Report No. DOE/ER/13955-17]
11. C. Pan, N.Y. Du, A.F. Starace, and C.H. Greene, CALCULATION OF THE PHOTODETACHMENT CROSS SECTION OF Li^- UP TO THE $4s$ THRESHOLD OF LITHIUM, Bull. Am. Phys. Soc. **38**, 1124 (1993). [DOE Report No. DOE/ER/13955-18]
12. I.I. Fabrikant, N.Y. Du, and A.F. Starace, ELECTRIC-FIELD EFFECTS IN H^- PHOTODETACHMENT WITH EXCITATION OF $H(n=2)$, Bull. Am. Phys. Soc. **38**, 1139 (1993). [DOE Report No. DOE/ER/13955-19]
13. N.Y. Du, A.F. Starace, and N.A. Cherepkov, RESONANT TWO-COLOR DETACHMENT OF H^- WITH EXCITATION OF $H(n=2)$, Abstracts of Contributed Papers, XVIII International Conference on the Physics of Electronic and Atomic Collisions, Vol. I, Edited by T. Andersen, B. Fastrup, F. Folkman, and H. Knudsen, Aarhus, Denmark, 21-27 July 1993, p. 107. [DOE Report No. DOE/ER/13955-20]

C. Reports

14. Progress Report (9/1/91 – 7/3/92) [DOE Report No. DOE/ER/13955-12]
15. Progress Report (8/1/92 – 7/31/93) [DOE Report No. DOE/ER/13955-15]
16. Progress Report (8/1/93 – 7/31/94) [DOE Report No. DOE/ER/13955-16]

IV. SUMMARY OF OVERALL PROGRESS

A. One- and Two-Photon Detachment of H^- with Excitation of $H(n=2)$ [Bibliography Item No. 1]

The cross sections for one- and two-photon detachment of H^- with excitation of the degenerate $H(2s)$ and $H(2p)$ levels have been calculated within an adiabatic hyperspherical representation. Both the partial cross sections, $\sigma(2s)$ and $\sigma(2p)$, and the photoelectron angular distribution asymmetry parameters were obtained. Our one-photon detachment results are dominated by the $^1P^o$ shape resonance feature above threshold, which is well known from prior theoretical and experimental work, with which our results were compared in detail. Our two-photon detachment cross sections and angular distribution asymmetry parameters exhibit a half-cycle of dipole-field-induced oscillation in the energy region from the $H(n=2)$ threshold to approximately 34 meV above threshold. The occurrence of a half-cycle of oscillation with significant amplitude over a 34-meV energy region above the $H(n=2)$ threshold is due to two circumstances unique to this two-photon process: first, in contrast to the strongly suppressed oscillations in the $^1S^e$ and $^1P^o$ attractive dipole-field channels for the $H(n=2)-e^-$ system, the amplitude of oscillation in the channel having $^1D^e$ symmetry is not strongly suppressed above threshold; second, electric dipole selection rules for the two-photon process do not permit population of the intense $^1P^o$ shape resonance located above the $H(n=2)$ threshold, which would otherwise obscure the half-cycle of dipole-field-induced oscillation. For these reasons, the process of two-photon detachment of H^- is a favorable one for observing this dipole-field-induced oscillation above threshold, which has yet to be observed experimentally in any process.

B. Long-Range Dipole Field Effects on H^- Detachment Processes Above the $H(n=2)$ Threshold [Bibliography Item No.2]

In this paper we show how the low-energy states of the fundamental $H(n=2) - e^-$ three-body system influence three very different processes for detaching the H^- ion. We also show that these three different detachment processes are each best suited to make manifest a different one of the properties of the long-range dipole field interactions within the $H(n=2) - e^-$ system. Thus, collisional detachment of H^- with measurement of the detached electron in the forward direction is best suited for demonstrating the finite threshold cross sections of those channels which have an attractive dipole-field interaction at asymptotic distances. This is so because the kinematic transformations from the projectile frame to the laboratory frame lead to a cusp behavior in the laboratory frame DDCS's which is possible only because of the finite threshold cross sections in the projectile frame.

Single photon detachment of H^- with excitation of $H(n=2)$ is ideal for observing the shape resonance feature in one of the $^1P^o$ final state channels above the $H(n=2)$ threshold. Electric dipole selection rules result in only final state channels having $^1P^o$ symmetry. The $^1P^+$ channel, in which the shape resonance occurs, has a cross section so much larger than those for other allowed $^1P^o$ channels that the shape resonance feature can be observed very clearly.

Finally, the two-photon detachment of H^- with excitation of $H(n=2)$ is the most likely process in which to observe the long-range dipole-field-induced oscillations above threshold that were predicted by Gailitis and Damburg but which have yet to be observed experimentally in any process. On the one hand, the $^1P^0$ shape resonance feature *is not* populated in this process, and hence cannot obscure these oscillations. On the other hand, the $^1D+$ final-state channel which *is* populated has the largest amplitude for such oscillations of any final state channel. Theoretical calculations predict a half cycle of such oscillation over the energy region from 0.1 meV to about 34 meV above threshold.

C. Hyperspherical Coordinate Description of Single- and Multiphoton Processes in Two-Electron Systems [Bibliography Item No. 3]

Much of our research that has been supported by DOE over many years was recently reviewed critically and placed in context with the theoretical work of others and with experimental measurements.

D. Variationally Stable Treatment of Two- and Three-Photon Detachment of H^- Including Electron-Correlation Effects [Bibliography Item No. 4]

We have recently presented a variationally stable, adiabatic hyperspherical treatment of two- and three-photon detachment of H^- . Results were compared with analytic predictions of a zero-range potential model of H^- . Detailed comparisons were made also with other theoretical results which include the effects of electron correlations. We predicted analytically (and demonstrated numerically) and extreme sensitivity of the theoretical predictions to any errors in the value of the electron affinity employed. We also showed that the low-intensity limit of the Keldysh treatment [Sov. Phys. JETP **20**, 1307 (1965)] of detachment of an electron bound in a zero-range potential agrees with the results of a perturbative treatment. Our calculated two- and three-photon detachment cross sections for H^- agree best with those of Mercouris and Nicolaides [Phys. Rev. A **45**, 2116 (1992)]. The results were recently found to be in excellent agreement with R-matrix results [J. Purvis et al., Phys. Rev. Lett. **71**, 3943 (1993)].

E. Resonant Two-Color Detachment of H^- with Excitation of $H(n=2)$ [Bibliography Item No. 5]

We have calculated the cross sections for resonant two-color, two-photon detachment of H^- with excitation of the degenerate $H(2s)$ and $H(2p)$ levels within a semiempirical adiabatic hyperspherical representation. The first photon, with energy $\omega_1 = 0.4017$ a.u., was chosen to be resonant with the well-known Feshbach $^1P^0$ resonance below the $H(n=2)$ threshold. The second photon, with energy $\omega_2 \geq 0.12605$ a.u., was chosen to scan the energy region above the $H(n=2)$ threshold over which long-range dipole-field-induced cross section oscillations are predicted to occur. Such Gailitis-Damburg oscillations have not yet been observed experimentally. Results for various pairs of light polarization for the two-photons were calculated. Our resonant two-color, two-photon detachment cross sections are 8-9 orders of magnitude greater than the corresponding nonresonant, single-color, two-photon detachment cross sections obtained by C.R. Liu, N.Y. Du, and A.F. Starace [Phys. Rev. A **43**, 5891 (1991)]. Unmistakable evidence of long-range dipole

field effects was demonstrated over the 5 meV energy range above the $H(n=2)$ threshold. Furthermore, the differential cross sections for right- and left-circularly polarized copropagating photons and especially the circular dichroism differential cross sections were found to have nearly a full cycle of a greatly enhanced dipole-field-induced oscillation extending over the region from threshold to ≈ 34 meV above.

F. Electric-Field Effects on H^- Photodetachment with Excitation of $H(n=2)$
[Bibliography Item No. 6]

A theory of the photodetachment of hydrogen negative ions in an external static electric field with the production of hydrogen in excited states was developed. We use a combination of the frame-transformation theory and the Green's-function method. The cross section in nonzero fields is expressed in terms of the photodetachment matrix elements for zero field. The latter were calculated using the adiabatic hyperspherical representation. For energies close to the threshold we use a smooth extrapolation of the zero-field photodetachment matrix elements down to threshold taking care to enforce the proper threshold behavior of cross sections for nonzero fields. The ripples in the *total* cross section due to interference effects are not noticeable for incident photons linearly polarized along the static field direction, but are relatively well pronounced for the case of circularly polarized photons propagating along the static field. On the other hand, all *partial* cross sections corresponding to photodetached electrons having magnetic quantum number $m' = 0$ (with respect to a quantization axis parallel to the static electric field) show significant ripple structure regardless of the light polarization. The partial cross section for detachment with excitation of the $n=2, m=1$ Stark substate by circularly polarized photons exhibits a particularly distinct ripple structure. All cross sections in the region of the shape resonance increase with increasing electric field in accordance with experimental observations. This effect is stronger in the case of linear polarization. We also predict a fairly stable value for the width of the $^1P^0$ shape resonance as a function of the electric-field strength over the range from 0.4 to 1 MV/cm. For electric-field strengths below 0.4 MV/cm, the ripple structure in the shape resonance makes it difficult to define a resonance width.

G. Parallels Between High Doubly-Excited State Spectra in H^- and Li^- Photodetachment [Bibliography Item No. 7].

Eigenchannel R-matrix calculations including effects of long-range multipole interactions outside the R-matrix box have been carried out for photodetachment of H^- and Li^- up to the $n=6$ threshold. Results for H^- give the first complete theoretical confirmation of experimental measurements [P.G. Harris et al, Phys. Rev. Lett. **65**, 309 (1990)] below the $n=5$ and $n=6$ thresholds. Partial cross sections for Li^- are found to be remarkably similar to those for H^- , despite the absence of atomic energy level degeneracy in the case of Li. Density plots for two electron resonances appearing in each spectrum confirm the similarity of the two spectra, indicating that advances in understanding doubly-excited states in two-electron systems have application to doubly-excited state spectra in many-electron systems. A more complete description of the present results, including presentation of the full spectrum for Li^- photodetachment from the $n=2$ to the $n=6$ thresholds, is being prepared for publication.

H. Photodetachment of $3P^e$ State of H^- [Bibliography Item No. 8].

The $3P^e$ state of H^- has been predicted theoretically to be bound below to the $H(n=2)$ threshold [cf. G.W.F. Drake, *Astrophys. J.* **184**, 145 (1973) and references therein]. However, it has never been observed experimentally. We have calculated the photodetachment cross section for this state using an adiabatic hyperspherical representation. The inverse process, the radiative capture process, may play a significant role in astrophysical plasmas. Its cross section is related to the photoionization process that we calculate by the Principle of Detailed Balance. Our results for detachment to the $H(2p)$ state and for the total $H(n=2)$ state agree well with the previous results of Jacobs, Bhatia, and Temkin [*Astrophys. J.* **242**, 1278 (1980)]. There is a disagreement for detachment to the $H(2s)$ state, however. This work is being prepared for publication.

**DATE
FILMED**

10 / 12 / 94

END