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Photodetachment of H^- in a static electric field

Arbitrary laser polarization direction

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Abstract. We derive a formula using closed-orbit theory for the photodetachment cross-section of H^- in the presence of a static electric field when there is an arbitrary angle θ_L between the laser polarization direction and the static electric field. This formula generalizes the previous result for laser polarization parallel to the static electric field, the effect of laser polarization direction appears as a factor $\cos^2(\theta_L)$ in the amplitude of the oscillation. A photodetachment cross-section formula valid above and below detachment threshold is proposed.

PACS. 32.60.+i Zeeman and Stark effects – 32.80.Gc Photodetachment of atomic negative ions – 31.15.Gy Semiclassical methods

Since Bryant et al. [1,2] observed the "ripple" structure in the photodetachment cross-section of H^- in the presence of a static electric field, photo-detachment of negative ions in a static electric field has attracted both theoretical and experimental attentions over the years [3–8]. Fabrikant studied the theories of photo-detachment of negative ions in a static electric field many years ago [9,10], Rau and Wong provided a first quantitative theory [11] for the observed "ripple" structure based on "Frame-transformation theory". Their photodetachment cross-section in an electric field involves an integral over Airy functions. Du and Delos [12] presented an alternative formula consisting of a smooth field-free background term and an oscillating term. Because this form is consistent with the more general closed-orbit theory [13–15], the "ripple" structure was interpreted as arising from the interference between the detached electron wave going out from and returning to the nucleus following a closed-orbit. A direct derivation of the two-term formula using closed-orbit theory was presented only recently [16].

Most of the discussions have focused on the case when the laser polarization direction is parallel to the static electric field direction, the "ripple" effect is the largest in this case and it has been experimentally observed [1,2]. When laser polarization direction is made perpendicular to the static electric field, the "ripple" effect in the photodetachment cross-section is very small [1,2], we have provided an explanation for the disappearance of oscillations [17]. What happens to the intermediate situation when there is an arbitrary angle θ_L between the laser polarization direction and the static electric field? In a study on photodetachment of negative ions in a static electric field with strong electromagnetic field, Ostrovsky and Telnov [18] were able to derive some general formulas for multi-photon detachment cross-sections. Their formula in their equation (7.5) does include a dependence on the angle between the electric field and the laser polarization direction. However, we note Ostrovsky and Telnov used several functions (such as A_n^0 and Γ_n^0 in their notations) in their formula, these functions are defined via integrals, but because they were concerned about general formulations, they did not consider any specific model for H^- in their paper, and they did not give explicit expressions for these functions. In contrast, we will consider a simple model for H^- and derive explicit expressions for the cross-section. Our approach is also very different from that of Ostrovsky and Telnov. We apply the standard closed-orbit theory [13–15] to this problem, closed-orbit theory has been very successful in describing the interferences in the photoinization of atoms in external fields in the last decade [15]. This approach allows us to follow the detached electron around various closed-orbits until it comes back to interfere. This approach enables us to clearly identify the physical origins of the different terms and factors in the cross-section [16]. In addition, we discuss how to extend our photodetachment formula below threshold, this problem was not considered by Ostrovsky and Telnov in their paper.

In this article we use a simple model for H^- and provide an quantitative answer to the question above. We follow the closed-orbit theory in reference [16] and derive a more general two-term formula in equation (14) for the photodetachment cross-section which is valid for an arbitrary laser polarization angle θ_L. In our new formula, the smooth background term is identical to the one in the parallel case [12,16], but for the oscillation term,

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while the phase of the oscillation remains the same as in the parallel case, the amplitude of the oscillation acquires an additional angle dependent factor $\cos^2(\theta_L)$, which normally reduces the oscillation. Atomic units will be used in the following. Because the present approach is similar to that in reference [16], we will only give the major steps and emphasize the differences in the derivations which are necessary for understanding the new result.

Assuming the static electric field in the z-direction and the laser polarization direction in (θ_L,ϕ_L). The photo-detached electron wave function ψ_d satisfies the schrödinger equation with a source term [16],

$$(E - H)\psi_d(\mathbf{r}) = D(\mathbf{r})\psi_i(\mathbf{r}) \quad (1)$$

where E is the energy of detached electron, ψ_i is the initial wave function of H^-, $\boldsymbol{\epsilon}$ is a unit vector in the direction of the laser polarization, $D(\mathbf{r}) = \mathbf{r}\cdot\boldsymbol{\epsilon}$ is the projection of electron coordinate on the direction of laser polarization direction. Following reference [12], we take the one electron approximation. The initial wave function in configuration space is then given by $\psi_i(\mathbf{r}) = Be^{-k_b r}/r$, B is a "normalization" constant and is equal to 0.31552, k_b has a numerical value 0.2355883, it is related to the binding energy E_b of H^- by $k_b = \sqrt{2E_b}$. H is the Hamiltonian governing the motion of the detached electron in the combined atomic potential $V_p(r)$ and the static electric field, it can be written as $H = \mathbf{p}^2/2 + V_p(r) + Fz$. Because the initial state is an S-state, the detached electron carries one angular momentum right after being detached near the nucleus, it is a good approximation to neglect $V_p(r)$ here.

The physical solution of equation (1) must be outgoing at large r. If the detached electron wave function $\psi_d(\mathbf{r})$ satisfying the correct outgoing boundary condition is obtained, the oscillator-strength density can be calculated by using the following formula [14]

$$Df(E,F,\theta_L) = -\frac{2(E_f - E_i)}{\pi}\mathrm{Im}\,\langle D(\mathbf{r})\psi_i|\psi_d\rangle. \quad (2)$$

The photodetachment cross-section is given by $\sigma(E,F) = (2\pi^2/c)Df(E,F,\theta_L)$, where c is the speed of light in au. Our formula for the oscillator-strength density in equation (2) together with the solution of the inhomogeneous equation (1) is equivalent to and derived [14] from the conventional oscillator-strength density formula involving the square of matrix elements in which the eigenfunctions for the detached electron have to be obtained. We solve equation (2) to get the detached electron wave function, which is a superposition of eigenfunctions.

To construct the solution of equation (1) near the nucleus using closed-orbit theory [13–15], the wave function $\psi_d(\mathbf{r})$ is separated into a direct part and a returning part, $\psi_d(\mathbf{r}) = (\psi_d)_{dir}(\mathbf{r}) + (\psi_d)_{ret}(\mathbf{r})$. The direct part represents the detached electron wave initially going out from the nucleus after photo-detachment and it satisfies the following equation

$$\left(E - \frac{\mathbf{p}^2}{2}\right)(\psi_d)_{dir} = D(\mathbf{r})\psi_i \quad (3)$$

which is obtained from equation (1) after dropping the static electric field term. The outgoing solution can be written in a more general form than the previous one [16]

$$(\psi_d)_{dir}(\mathbf{r}) = -\frac{4Bk^2 i}{(k_b^2 + k^2)^2}h_1^{(1)}(kr)f(\theta,\phi;\theta_L,\phi_L) \quad (4)$$

where $k = \sqrt{2E}$ is the momentum of the detached electron, $h_1^{(1)}(kr)$ is the outgoing spherical Bessel function [19,20], and

$$f(\theta,\phi;\theta_L,\phi_L) = \cos(\theta)\cos(\theta_L) + \sin(\theta)\sin(\theta_L)\cos(\phi - \phi_L) \quad (5)$$

represents the dependence of the detached electron wave function on the outgoing direction (θ,ϕ). The overlap integral of the direct part with the source gives the same smooth field-free background term [12,16],

$$Df_0(E) = -\frac{2(E_f - E_i)}{\pi}\mathrm{Im}\,\langle D(\mathbf{r})\psi_i|(\psi_d)_{dir}\rangle = \frac{8\sqrt{2}B^2E^{3/2}}{3(E_b + E)^3}. \quad (6)$$

There are two methods to calculate this overlap integral. In the first method, the variables in the integral are rewritten in a coordinate system with its z-axis pointing to the laser direction, the integral then becomes identical to the parallel case [16]. In the second method, we relate this overlap integral to the integrated outgoing electron flux [19] when there is no static electric field. It is clear that this integrated outgoing flux is independent of the laser polarization direction, the above overlap integral is therefore equal to that obtained earlier [16].

For the oscillation term, we have to follow the detached electron wave first going away from the nucleus along the z-axis and later returning back to the nucleus. The electron follows a closed-orbit. The wave function $(\psi_d)_{ret}(\mathbf{r})$ represents the electron wave near the nucleus when it is back. Physically $(\psi_d)_{ret}(\mathbf{r})$ is the continuation of $(\psi_d)_{dir}(\mathbf{r})$ along the closed-orbit. To obtain the returning wave function associated with the closed-orbit, we draw a sphere of radius R, R is large enough so that the asymptotic approximation $h_1^{(1)}(kr) = e^{i(kr-\pi)}/kr$ is valid, it also must be small enough so that the electric field potential term is much smaller than the initial kinetic energy term of the detached electron inside the sphere, that is, $zF \ll k^2/2$. In our case, the direct outgoing wave on the surface of this sphere is

$$(\psi_d)_{dir}(\mathbf{r}) = -i\frac{4Bk^2}{(k_b^2 + k^2)^2}f(\theta,\phi;\theta_L,\phi_L)\frac{e^{i(kr-\pi)}}{kr}. \quad (7)$$

The returning wave near the nucleus can be approximated by a plane wave traveling in the negative z-direction,

$$(\psi_d)_{ret}(\mathbf{r}) = ge^{-ikz}, \quad (8)$$

and

$$g = Ae^{i(S-\frac{\pi}{2})}(\psi_d)_{dir}(\theta = 0, R), \quad (9)$$

where S is a phase integral $\int \mathbf{p}d\mathbf{q}$ along the closed orbit from the surface out and back to the origin $\mathbf{q} = 0$, $\pi/2$ is the phase correction at the turning point of the closed-orbit, A is a measure of the amplitude of the returning wave. In the present problem, $(\psi_d)_{dir}(\theta = 0, R)$ is different from the parallel polarization, but we can still use the previous S and A [16,19],

$$A = \sqrt{\frac{R^2 k}{(R+kt)^2|k - ft\cos(\theta_i)|}} \quad (10)$$

where t is the time going from the surface out and back to the origin, θ_i is the outgoing direction of the closed-orbit and is zero here. When the expression in equation (10) is used in equation (9) and the limit of small R is taken, we get

$$g = \frac{2BFi}{k(k_b^2 + k^2)^2} e^{i(S-\pi/2)} \cos(\theta_L), \quad (11)$$

where

$$S = \frac{4\sqrt{2}E^{3/2}}{3F} \quad (12)$$

is the action integral around the closed-orbit.

The overlap integral of the returning wave with the source gives the oscillation term in the oscillator-strength density,

$$\begin{aligned} Df_1(E, F, \theta_L) &= -\frac{2(E_f - E_i)}{\pi} \mathrm{Im}\,\langle D(\mathbf{r})\psi_i | (\psi_d)_{ret} \rangle \\ &= \frac{2FB^2}{(E_b + E)^3} \cos^2(\theta_L)\cos(S). \end{aligned} \quad (13)$$

The overlap integral can be evaluated in the following way. We first write $D(\mathbf{r}) = D_1(\mathbf{r}) + D_2(\mathbf{r})$ where $D_1(\mathbf{r}) = r \cos(\theta)\cos(\theta_L)$ and $D_2(\mathbf{r}) = r\sin(\theta)\sin(\theta_L)\cos(\phi - \phi_L)$, the overlap integral in equation (13) is split into two integrals corresponding to D_1 and D_2. The integral corresponding to D_1 differs from the integral in equation (11) of reference [16] by $\cos^2(\theta_L)$, the integral corresponding to D_2 is zero because both $\psi_i(\mathbf{r})$ and $(\psi_d)_{ret}(\mathbf{r})$ are independent of the variable ϕ but D_2 changes sign when ϕ is increased by π. When equations (6) and (13) are combined, we have the final formula for the photodetachment cross-section in an electric field with an angle θ_L between the laser polarization direction and the static electric field above threshold

$$\begin{aligned} \sigma(E, F, \theta_L) &= \frac{16\sqrt{2}B^2\pi^2 E^{3/2}}{3c(E_b + E)^3} \\ &\quad + \frac{4B^2\pi^2 F}{c(E_b + E)^3} \cos^2(\theta_L)\cos(S), \quad E \geq 0 \end{aligned} \quad (14)$$

where [21] $c = 137.037$ and the numerical value for B is given right after equation (1). The first term on the right side of equation (14) is the total detached outgoing electron flux neglecting the electric field, the second term is the interference in the detachment cross-section induced by the outgoing electron wave and the group of returning electron wave, which first propagates away from the negative ion in the electric field direction and later returns back to the negative ion following a closed-orbit, the sign of the interference is determined by the phase accumulation S, the factor $\{(4B^2\pi^2 F)/[c(E_b + E)^3]\}\cos^2(\theta_L)$ is the electron emission amplitude multiplied by the recombination amplitude, in which $\cos^2(\theta_L)$ is the angular dependence. We emphasize that this square dependence is really a special case of this problem. In other problems such as atoms in a magnetic field [13–15], the initial outgoing angle and the final returning angle of an electron closed-orbit can be different, then a more complicated angular dependence is obtained.

We can now better understand the dependence of photodetachment cross-section on laser polarization direction. The formula for the parallel polarization case obtained earlier [12,16] is just a special case of the present formula in equation (14) with $\theta_L = 0$. It corresponds to the largest oscillation, the "ripple" effect is therefore more visible. When the laser polarization is perpendicular to the static electric field, $\theta_L = \pi/2$, equation (14) predicates the oscillation amplitude to be zero. The observed "ripple" effect is not zero but very small [1,2], which is consistent with our earlier quantum theory [12,17] for the perpendicular polarization case. The present semiclassical theory for the perpendicular polarization case can be refined by assuming a more accurate outgoing wave function $\psi_d(\mathbf{r})$ when it is in a node [23], but it is beyond the scope of the present article. For any other angle, the oscillation amplitude is between the above two extreme values and it can be calculated readily using equation (14). For example, it is easy to predict the oscillation amplitude should be reduced to a half when the laser polarization angle is increased from $\theta_L = 0$ (parallel case) to $\theta_L = \pi/4$. For $E \geq 0$, the $\cos^2(\theta_L)$ factor in the oscillation amplitude is a direct reflection of the intensity of the returning wave near the nucleus [17] when the angle is varied. The present formula should be accurate away from $\theta_L = \pi/2$.

The formula in equation (14) can be written more compactly as

$$\sigma(E, F, \theta_L) = \sigma_0(E)\left[1 + \cos^2(\theta_L)\frac{\cos(S)}{S}\right], \quad E \geq 0 \quad (15)$$

where S is related to E and F in equation (12) and

$$\sigma_0(E) = \frac{16\sqrt{2}B^2\pi^2 E^{3/2}}{3c(E_b + E)^3} \quad (16)$$

is the photodetachment cross-section in the absence of a static electric field. This formula in equation (15) suggests that E and S are better variables than E and F for analyzing the oscillation in the cross-section. This scaling in the detachment cross-section was already noticed by Fabrikant [9,10,22]. Suppose we can measure or numerically compute $\sigma(E, F, \theta_L)$. Defining the Fourier transformation by $\hat{\sigma}(w) = \int_{S_l}^{S_r} [\sigma(E, F, \theta_L)/\sigma_0(E)] \exp(-iwS) S dS$ and assuming $(S_r - S_l) \gg 2\pi$, we expect the absolute value of $\hat{\sigma}(w)$ as a function of w for any θ_L should display a peak at $w = 1$, and the peak height should be equal

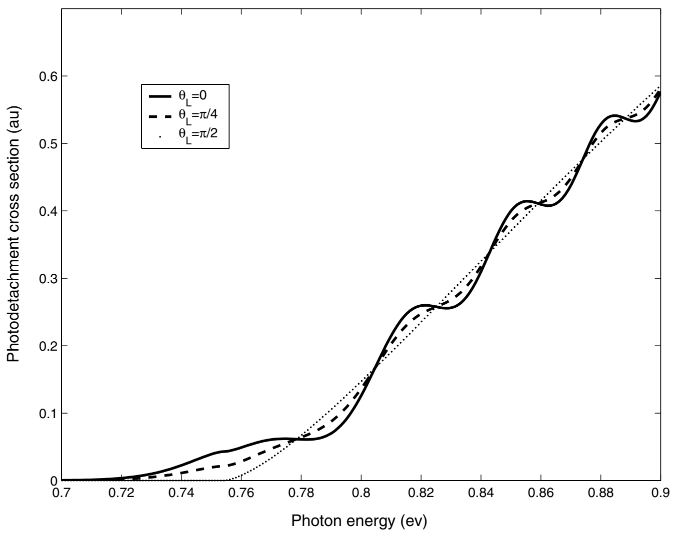

Fig. 1. Theoretical photodetachment cross-sections given in equations (14) and (17) for H^- in a static electric field $F = 164$ kV/cm with three different laser polarization angles relative to the static electric field direction. Solid lines: $\theta_L = 0$, dashed lines: $\theta_L = \pi/4$ and dotted lines: $\theta_L = \pi/2$.

to $(S_r - S_l)\cos^2(\theta_L)/2$ according to out present theory. This provides a way to verify the effect of laser polarization direction on the photodetachment cross-section in the presence of a static electric field.

For energy $E \leq 0$, we have shown the cross-section is an exponential function in the parallel polarization case [12]. Due to its asymptotic nature, however, the formula for $E \leq 0$ and the formula for $E \geq 0$ do not smoothly match at $E = 0$. One may fix this problem by adjusting the pre-exponential constant for $E \leq 0$ so it smoothly joins the formula for $E \geq 0$ [24]. In our present problem, the laser polarization is at an angle θ_L with the static electric field, we argue an angle dependent factor $\cos^2(\theta_L)$ similar to the second term of equation (14) should appear in the pre-exponential constant because for $E \leq 0$ the major contribution comes from the detached electron tunneling in the negative static electric field direction. The suggested formula for $E \leq 0$ is therefore

$$\sigma(E, F, \theta_L) = \frac{4B^2\pi^2 F}{c(E_b + E)^3}\cos^2(\theta_L) \times \exp\left(-\frac{4\sqrt{2}(-E)^{3/2}}{3F}\right), \quad E \leq 0. \quad (17)$$

In Figure 1 we show the cross-sections described by equations (14) and (17) for $\theta_L = 0$, $\pi/4$ and $\pi/2$. It gives an overall good description for the cross-section below and above threshold. In the parallel polarization case and above threshold, this formula slightly over estimates the cross-section near $E = 0$ when it is compared with the quantum result [12]. This deviation near $E = 0$ should not be surprising because in our derivation we have made the approximation that the outgoing wave is the same as the one without the electric field. For this approximation to be valid, it is required that $zF \ll k^2/2$. If z is taken as $10a$ and $F = 164$ kV/cm is used as in Figure 1, the value of the left hand side of the inequality is about 0.01 eV. Therefore our formula in equation (14) is expected to be accurate above threshold by a few 0.01 eV.

In summary, we have applied closed-orbit theory and derived a more general formula in equations (14) and (17) describing the photodetachment cross-section of H^- in the presence of a static electric field when there is an arbitrary angle θ_L between the laser polarization and the static electric field. This formula gives a special simple dependence of the cross-section on the polarization angle. We hope this theoretical prediction will stimulate future experiments on this question.

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References

1. H.C. Bryant, A. Mohagheghi, J.E. Stewart, J. Donahue, C.R. Quick, R.A. Reeder, V. Yuan, C. Hummer, W.W. Smith, S. Cohen, et al., Phys. Rev. Lett. **58**, 2412 (1987)
2. J.E. Stewart, H.C. Bryant, P.G. Harris, A.H. Mohagheghi, J.B. Donahue, C.R. Quick, R.A. Reeder, V. Yuan, C.R. Hummer, W.W. Smith, et al., Phys. Rev. A **38**, 5628 (1988)
3. N.D. Gibson, B.J. Davis, D.J. Larson, Phys. Rev. A **47**, 1946 (1993)
4. N.D. Gibson, B.J. Davis, D.J. Larson, Phys. Rev. A **48**, 310 (1993)
5. C. Rangan, A.R.P. Rau, Phys. Rev. A **61**, 033405 (2000)
6. N.D. Gibson, M.D. Gasda, K.A. Moore, D.A. Zawistowski, C.W. Walter, Phys. Rev. A **64**, 061403(R) (2001)
7. I.I. Fabrikant, M.V. Frolov, N.L. Manakov, A.F. Starace, Phys. Rev. A **64**, 037401 (2001)
8. A.R.P. Rau, C. Rangan, Phys. Rev. A **64**, 037402 (2001)
9. I.I. Fabrikant, Sov. Phys. JETP **52**, 1045 (1980)
10. I.I. Fabrikant, Sov. Phys. JETP **56**, 967 (1982)
11. A.R.P. Rau, H. Wong, Phys. Rev. A **37**, 632 (1988)
12. M.L. Du, J.B. Delos, Phys. Rev. A **38**, 5609 (1988)
13. M.L. Du, J.B. Delos, Phys. Rev. Lett. **58**, 1731 (1987)
14. M.L. Du, J.B. Delos, Phys. Rev. A **38**, 1896 (1988); M.L. Du, J.B. Delos, Phys. Rev. A **38**, 1913 (1988)
15. A. Matzkin, P.A. Dando, T.S. Monteiro, Phys. Rev. A **66**, 013410 (2002); D. Kleppner, J.B. Delos, Found. Phys. **31**, 593 (2001) and references therein; B.E. Granger, C.H. Greene, Phys. Rev. A **62**, 012511 (2000) and references therein
16. M.L. Du, Phys. Rev. A **70**, 055402 (2004)
17. M.L. Du, J.B. Delos, Phys. Lett. A **134**, 476 (1989)
18. V.N. Ostrovsky, D.A. Telnov, J. Phys. B **26**, 415 (1993)
19. M.L. Du, Phys. Rev. A **40**, 4983 (1989)
20. *Handbook of Mathematical Functions*, edited by M. Abramowitz, I.A. Stegun (Dover, New York, 1987)
21. H.A. Bethe, E.E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum, New York, 1977)
22. I.I. Fabrikant, Phys. Rev. A **40**, 2373 (1989)
23. J.A. Shaw, J.B. Delos, M. Courtney, D. Kleppner, Phys. Rev. A **51**, 3695 (1995)
24. H.C. Bryant, J. Chin. Chem. Soc. **48**, 333 (2001)