

Photodetachment of H^- in an electric field

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(Received 25 April 1988)

A simple analytic formula for the photodetachment cross section of H^- in an electric field is derived. The formula becomes identical to a formula derived many years ago in the vanishing-field limit. Three special features appear in the cross section in the presence of an electric field: a quantum tunneling effect, a new threshold law, and oscillations. These appear when the photon energy is, respectively, less than, equal to, or greater than the binding energy of H^- . Enough information is provided in this paper so that one can calculate the cross section quickly.

I. INTRODUCTION

Very recently, experimental measurements were made of the cross section for photodetachment from H^- , $h\nu + H^- \rightarrow H + e^-$, in static external electric fields of a few hundred kV/cm.¹ Near the detachment threshold ($h\nu = 0.7542$ eV) a "ripple" structure was found in the cross section as a function of energy. This is quite different from the smooth photodetachment cross section that occurs in the absence of any field.

Our aim in this paper is to explain and interpret these observations. We will derive a simple formula for the photodetachment cross section of H^- in an electric field. The formula is found to be quite accurate, and very easy to use.

The photodetachment cross section is related to a dipole matrix element, which we write in "velocity form." In the initial bound state, H^- is regarded as effectively a one-electron system, with the electron loosely bound by a short-range potential. The effect of the electric field on the initial state can be ignored, since in the initial bound state the external field strength is very small compared to the atomic field strength. The wave functions for the motion of the electron after detachment are the wave functions of an electron in an electric field only, and the effect of the short-range potential of the atomic core is ignored after the electron is detached. This is appropriate since (in the absence of the electric field) photoabsorption causes a transition from an S to a P state; in the final state the electron stays well away from the atomic core, outside of the P -wave centrifugal barrier (i.e., the radial wave function associated with a P state goes to zero at the origin). Therefore the contribution of the atomic core region to the dipole matrix element is small.² It also follows from this argument that our approximation to the initial state only needs to be accurate outside of the atomic core.

These approximations turn out to be surprisingly accurate. Similar approximations were used long ago to calculate photodetachment cross sections in the absence of external fields,³ and the agreement with experiment

turned out to be very good—even better than that obtained from a 20-parameter variational calculation. (Similar approximations have also been used to study above-threshold detachment in intense laser fields.⁴)

In Sec. II the photodetachment cross section is derived from the wave functions in momentum space. Then in Sec. III a function $D(x)$ appearing in the formula is studied in greater detail. Information is provided to evaluate the function $D(x)$ and the cross section quickly. Discussion of the features in the cross section is given in Sec. IV, and comparison with experiment in Sec. V. Atomic units are used throughout this paper unless otherwise noted.

After this work was essentially complete, we learned that Rau and Wong⁵ obtained one of the formulas from "frame-transformation theory." Our derivation is simpler and more direct; we reduce the formula to one suitable for a pocket calculator, we give more detail about the cross sections, and we give a correct value for a rather confusing constant that appears in the theory.

II. DERIVATION

Let the energy of the escaping electron be denoted by $E = \hbar^2 k^2 / 2m_e$, the binding energy of the electron to the negative ion by $E_b = 0.754$ eV, and the photon energy by $E_p = E + E_b$. The photodetachment cross section in the presence of electric field F , $\sigma(E, F)$, is related to an oscillator-strength density $Df(E, F)$ by

$$\sigma(E, F) = (2\pi^2 e^2 \hbar / m_e c) Df(E, F), \quad (1)$$

where

$$Df(E, F) = \int (2m_e E_p / \hbar^2) |\langle f | z | i \rangle|^2 \delta(E(f) - E) df \quad (2a)$$

$$= \int \left[\frac{2}{m_e E_p} \right] |\langle f | p_z | i \rangle|^2 \delta(E(f) - E) df. \quad (2b)$$

Here $\langle f |$ represents any final state, normalized such that $\langle f | f' \rangle = \delta(f - f')$. The total photodetachment cross section is an incoherent sum of cross sections to each dis-

tinct final state. In Eq. (2) it is assumed that the electric field of the laser is polarized along the z axis (c is the speed of light, equal to 137 a.u.).

We take the initial wave function in configuration space to be

$$\psi_i(\mathbf{q}) = B \frac{e^{-k_b r}}{r}, \quad (3)$$

where k_b is related to the binding energy E_b of H^- by

$$E_b = \frac{k_b^2}{2}. \quad (4)$$

The best value extracted from a variational calculation is³

$$k_b = 0.235\,5883. \quad (5)$$

The constant B needs to be determined with care: in the Appendix we explain why its value should be taken to be

$$B = 0.315\,52. \quad (6)$$

The corresponding wave function ψ_i in momentum space is

$$\psi_i(\mathbf{p}) = B \left[\frac{2}{\pi} \right]^{1/2} \frac{1}{(k_b^2 + p^2)}. \quad (7)$$

If the static electric field also points in the z direction, then the wave functions in momentum space for an electron moving in this field satisfy

$$\left[\frac{\mathbf{p}^2}{2} + iF \frac{\partial}{\partial p_z} \right] \psi_f = E \psi_f. \quad (8)$$

Any particular one of these final states, $\psi_{f'}$, can be labeled by three conserved quantities—the energy E'_z associated with z motion and the momentum (p'_x, p'_y) associated with x and y motion:

$$f' \leftrightarrow (p'_x, p'_y, E'_z),$$

$$\psi_{f'}(\mathbf{p}) = \delta(p_x - p'_x) \delta(p_y - p'_y) (2\pi F)^{-1/2}$$

$$\times \exp \left[\left[\frac{i}{F} \right] \left[\frac{p_z^3}{6} - E'_z p_z \right] \right]. \quad (9)$$

These wave functions are normalized according to

$$\int \psi_{f'}(\mathbf{p}) \psi_{f''}(\mathbf{p}) d\mathbf{p} = \delta(p'_x - p''_x) \delta(p'_y - p''_y) \delta(E'_z - E''_z). \quad (10)$$

Therefore the dipole matrix element (2b) is

$$\begin{aligned} \langle \psi_i | p_z | \psi_{f'} \rangle &= \int d\mathbf{p} \left\{ \delta(p_x - p'_x) \delta(p_y - p'_y) (2\pi F)^{-1/2} \exp \left[\left[\frac{i}{F} \right] \left[\frac{p_z^3}{6} - E'_z p_z \right] \right] p_z B \left[\frac{2}{\pi} \right]^{1/2} \left[\frac{1}{k_b^2 + p^2} \right] \right\} \\ &= \frac{B}{\pi F^{1/2}} \int dp_z \frac{1}{(k_b^2 + p_x'^2 + p_y'^2 + p_z^2)} p_z \exp \left[\left[\frac{i}{F} \right] \left[\frac{p_z^3}{6} - E'_z p_z \right] \right]. \end{aligned} \quad (11)$$

The major contributions to the above integral come from the stationary phase points p_z satisfying

$$\frac{p_z^2}{2} - E'_z = 0. \quad (12)$$

Because the initial wave function $\psi_i(\mathbf{p})$ is slowly varying around the stationary phase points, we evaluate it at the stationary phase points and take it outside the integral. Thus we obtain

$$\begin{aligned} \langle \psi_i | p_z | \psi_{f'} \rangle &= \frac{B}{\pi} \frac{1}{\sqrt{F}} \frac{1}{(k_b^2 + p^2)} \left[\frac{F}{-i} \right] \frac{\partial}{\partial E'_z} \int_{-\infty}^{\infty} dp_z \exp \left[\left[\frac{i}{F} \right] \left[\frac{p_z^3}{6} - E'_z p_z \right] \right] \\ &= iB 2^{4/3} F^{5/6} \frac{1}{(k_b^2 + p^2)} \frac{\partial}{\partial E'_z} \text{Ai} \left[- \left[\frac{2}{F^2} \right]^{1/3} E'_z \right] \end{aligned} \quad (13)$$

and

$$\begin{aligned} Df(E, F) &= \frac{2}{(E + E_b)} \int |\langle \psi_i | p_z | \psi_f \rangle|^2 \delta \left[E - \frac{p_x'^2}{2} - \frac{p_y'^2}{2} - E'_z \right] dp'_x dp'_y dE'_z \\ &= \frac{64\pi B^2 F}{(k_b^2 + p^2)^3} D \left[\frac{2^{1/3} E}{F^{2/3}} \right], \end{aligned} \quad (14)$$

where $D(x)$ is a function defined by

$$D(x) \equiv \int_{-\infty}^x \left[\frac{d}{dz} \text{Ai}(-z) \right]^2 dz. \quad (15)$$

$\text{Ai}(z)$ is the standard Airy function.⁶

Hence the photodetachment cross-section is

$$\begin{aligned} \sigma(E, F) &= \frac{128\pi^3}{c} \frac{B^2 F}{(k_b^2 + p^2)^3} D(2^{1/3} E / F^{2/3}) \\ &= 0.3604 \frac{F}{(E_b + E)^3} D(2^{1/3} E / F^{2/3}) a_0^2, \end{aligned} \quad (16)$$

where, again, F is the electric field in atomic units (1 a.u. electric field = 5.14×10^9 V/cm), E is the energy of the detached electron, and E_b is the binding energy of the initial state.

III. THE FUNCTION $D(x)$

In this section we discuss the function $D(x)$ appearing in the cross-section formula (16). As we shall see, the structure of the observed cross section is contained almost entirely in this function $D(x)$.

The function $D(x)$ is defined in (15). For convenience, we rewrite the definition in the form

$$D(x) \equiv \int_{-\infty}^x \left[\frac{d}{dz} \text{Ai}(-z) \right]^2 dz = \int_{-x}^{\infty} \left[\frac{d}{dz} \text{Ai}(z) \right]^2 dz. \quad (17)$$

$D(x)$ is positive everywhere. The Airy function satisfies the differential equation

$$\frac{d^2}{dz^2} \text{Ai}(z) - z \text{Ai}(z) = 0, \quad (18)$$

with asymptotic condition at large positive z ,

$$\text{Ai}(z) \sim \frac{1}{2\sqrt{\pi}} z^{-1/4} \exp(-\frac{2}{3}z^{3/2}), \quad z \rightarrow \infty. \quad (19)$$

Consider first the region where x is very negative. Then the asymptotic approximation (19) to the Airy function can be used, and after integration, one easily obtains

$$D(x) = \frac{1}{8\pi} \exp[-\frac{4}{3}(-x)^{3/2}], \quad x \leq -4.75. \quad (20)$$

This approximation is found to have an error of 2% at $x = -4.75$, and the error becomes smaller for more negative x .

To evaluate the function $D(x)$ numerically, one can integrate three coupled first-order differential equations. Defining

$$u(z) = \text{Ai}(z), \quad (21a)$$

$$v(z) = d \text{Ai}(z) / dz, \quad (21b)$$

$$w(z) = D(-z), \quad (21c)$$

it is evident that u , v , and w satisfy the differential equations

$$du(z)/dz = v(z), \quad (22a)$$

$$dv(z)/dz = zu(z), \quad (22b)$$

$$dw(z)/dz = -v(z)^2, \quad (22c)$$

with initial conditions at large z

$$u(z) = \frac{1}{2\sqrt{\pi}} z^{-1/4} \exp(-\frac{2}{3}z^{3/2}), \quad (23a)$$

$$v(z) = -\frac{1}{2\sqrt{\pi}} z^{1/4} \exp(-\frac{2}{3}z^{3/2}), \quad (23b)$$

$$w(z) = \frac{1}{8\pi} \exp(-\frac{4}{3}z^{3/2}). \quad (23c)$$

Integration is performed from large positive to large negative z .

Finally, for large positive x ($x \geq 4.0$), the oscillatory asymptotic approximation

$$\text{Ai}(-z) \sim \pi^{-1/2} z^{-1/4} \sin(\frac{2}{3}z^{3/2} + \pi/4) \quad (24a)$$

can be used, from which we obtain

$$\left[\frac{d \text{Ai}(-z)}{dz} \right]^2 \sim \frac{1}{2\pi} z^{1/2} \left[1 + \cos \left[\frac{4}{3}z^{3/2} + \frac{\pi}{2} \right] \right]. \quad (24b)$$

After integration we find

$$D(x) = \frac{1}{4\pi} \left[\frac{4}{3}x^{3/2} + \cos(\frac{4}{3}x^{3/2}) \right] \quad (25)$$

plus an undetermined constant of integration. By comparison of this formula with the results of numerical integration, we find that the constant should be taken to be zero.

This approximation becomes better for large positive x . Actually it is a surprisingly good approximation for all positive x ; for example, at $x = 4.0$, the error in the approximation is only 0.2%.

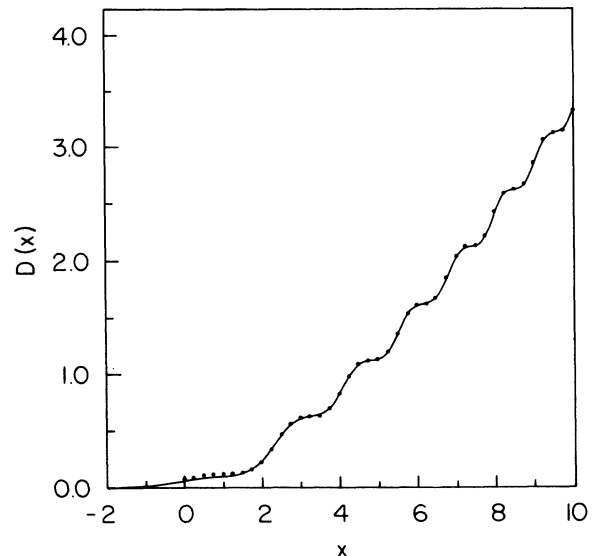


FIG. 1. The function $D(x)$. Solid line is the numerical result, from integration. The dots are approximation (25).

Approximations (19) for negative x and (25) for positive x do not match at $x=0$. A table of numerically determined values of $D(x)$ is provided for this intermediate region. With this table and the approximations in the other two regions, the function $D(x)$ is easily evaluated.

A graph of $D(x)$ is shown in Fig. 1. Also shown is the approximation (25). One can see that $D(x)$ increases from an exponentially small value at negative x to a finite value of $x=0$, and it becomes increasingly large and oscillatory as x increases.

From these properties of the function $D(x)$, we shall obtain the characteristics of the photodetachment cross section for H^- in an electric field in the next section.

IV. THE CROSS SECTION

Three special phenomena exist in the cross section when an electric field is present. Below the (zero-field) detachment threshold, detachment occurs by tunneling. At the threshold, the photodetachment cross section has a finite value which is proportional to the electric field strength. Above threshold, this cross section is oscillatory. All these phenomena are described quantitatively by the formula (16).

First let us verify that Eq. (16) approaches the correct limit as the electric field strength F goes to zero. For photon energy smaller than the binding energy, that is, for E less than zero, as $F \rightarrow 0$, the argument of function $D(x)$ in (16) goes to minus infinity. Therefore approximation (20) can always be used. Clearly we obtain

$$\sigma(E < 0, F \rightarrow 0) \rightarrow 0. \quad (26)$$

On the other hand, if the photon energy is greater than the binding energy, so E is positive, then as $F \rightarrow 0$, the argument of function $D(x)$ in Eq. (16) goes to positive infinity. Then approximation (25) can be used. Now since x goes to infinity the second term in Eq. (25) is very small compared with the first term (and rapidly oscillatory as well), so it can be dropped. We then obtain

$$\begin{aligned} \sigma(E > 0, F \rightarrow 0) &\rightarrow \frac{16\sqrt{2}B^2\pi^2}{3c} \frac{E^{3/2}}{(E_b + E)^3} a_0^2 \\ &\rightarrow 0.05408 \frac{E^{3/2}}{(E_b + E)^3} a_0^2. \end{aligned} \quad (27)$$

This is identical to the formula given by Ohmura and Ohmura,³ except that we are using atomic units here. This formula contains within it the Wigner threshold law, $\sigma \propto E^{3/2}$, appropriate for p -wave electrons.

Now turning on the electric field, we compute photodetachment cross sections from Eq. (16). The results are shown in Fig. 2 for three different values of the electric field strength F . Special features appearing in the cross sections are discussed now in order.

For photon energy smaller than the binding energy of H^- , in the absence of the electric field, the photodetachment cross section is zero. As soon as the field is present, the cross section becomes nonzero, but still it is exponentially small. This small cross section may be regarded as a quantum tunneling effect: even for energies below the

zero-field threshold, the electron can tunnel out through a potential-energy barrier, and go to the downhill side of the potential energy. From (16) and (20) we obtain the

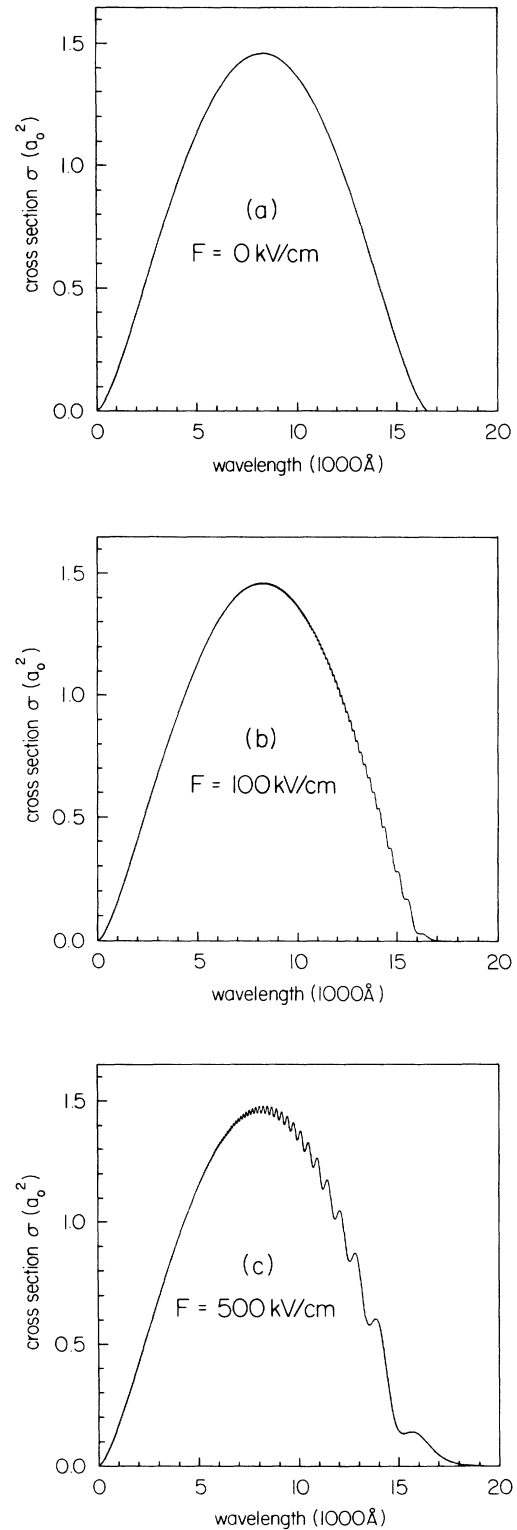


FIG. 2. Photodetachment cross sections as a function of photon wavelength (a) for electric field $F=0$, (b) for $F=100$ kV/cm, and (c) for $F=500$ kV/cm.

cross section in the tunneling region,

$$\begin{aligned}\sigma(E, F) &= \left[\frac{2\pi^2 B^2}{c} \right] \frac{F}{(E_b + E)^3} \exp \left[-\frac{4\sqrt{2}}{3F} (-E)^{3/2} \right] a_0^2 \\ &= 0.01434 \frac{F}{(E_b + E)^3} \exp \left[-\frac{4\sqrt{2}}{3F} (-E)^{3/2} \right] a_0^2.\end{aligned}\quad (28)$$

Exactly at threshold, in the absence of an external field, the photodetachment cross section is again zero. In the presence of a field, however, from Table I we find $D(x=0)=0.06117$, and therefore we find that the detachment cross section is proportional to the electric-

TABLE I. Function $D(x)$. The number in square brackets is the power of ten to which the number is raised ($4.12[-8]=4.12 \times 10^{-8}$).

x	$D(x)$
-4.75	4.12 [-8]
-4.50	1.21 [-7]
-4.25	3.45 [-7]
-4.00	9.55 [-7]
-3.75	2.56 [-6]
-3.50	6.66 [-6]
-3.25	1.67 [-5]
-3.00	4.07 [-5]
-2.75	9.55 [-5]
-2.50	2.16 [-4]
-2.25	4.70 [-4]
-2.00	9.82 [-4]
-1.80	1.72 [-3]
-1.60	2.92 [-3]
-1.40	4.83 [-3]
-1.20	7.74 [-3]
-1.00	1.20 [-2]
-0.80	1.80 [-2]
-0.60	2.60 [-2]
-0.40	3.60 [-2]
-0.20	4.80 [-2]
0.00	6.12 [-2]
0.20	7.43 [-2]
0.40	8.58 [-2]
0.60	9.41 [-2]
0.80	9.83 [-2]
1.00	9.91 [-2]
1.20	9.98 [-2]
1.40	1.06 [-1]
1.60	1.25 [-1]
1.80	1.65 [-1]
2.00	2.30 [-1]
2.20	3.16 [-1]
2.40	4.13 [-1]
2.60	5.04 [-1]
2.80	5.72 [-1]
3.00	6.08 [-1]
3.20	6.17 [-1]
3.40	6.19 [-1]
3.60	6.43 [-1]
3.80	7.11 [-1]
4.00	8.22 [-1]

field-strength,

$$\sigma(E=0, F) = 1.032 \times 10^3 F a_0^2. \quad (29)$$

Usually this gives a small cross section. For example, for a field as strong as 10^6 V/cm, the cross section is only $0.2a_0^2$.

The most interesting region of the cross section is where the photon energy is greater than the binding energy. In this region, oscillations appear in the cross section. To see these explicitly, let us use approximation (25) for the function $D(x)$. The cross section, Eq. (16), is then a sum of two terms,

$$\begin{aligned}\sigma(E, F) &= 0.05408 \frac{E^{3/2}}{(E_b + E)^3} \\ &+ 0.02868 \frac{F}{(E_b + E)^3} \cos \left[\frac{4\sqrt{2}E^{3/2}}{3F} \right] a_0^2.\end{aligned}\quad (30)$$

The first term in Eq. (30) is independent of the field strength [in fact, it is Eq. (27) for the cross section when there is no field]. The second term is an oscillatory term. The amplitude of the oscillations is proportional to the electric field strength, and it decreases as the photon energy increases. The wavelength of the oscillations is inversely proportional to the electric field strength so as the field increases, the peaks of the oscillations become more clearly visible.

One sees from the formula (30) that the net contribution of the electric field to the photodetachment cross-section is small. The oscillations are substantial only close to the threshold. Above threshold, if we average over the oscillations, the zero-field result is obtained.⁷

Positions of maxima and minima are trivially predicted. The energy of the n th maximum or minimum in the cross section above threshold is approximately given by the energy of the corresponding maximum or minimum of the cosine term in Eq. (30):

$$E_{\max}^n = \frac{1}{2} [3\pi F(n-1)]^{2/3}, \quad (31a)$$

$$E_{\min}^n = \frac{1}{2} [3\pi F(n-\frac{1}{2})]^{2/3}. \quad (31b)$$

Comparing with the numerically determined cross sections, these positions are accurate, except for the first peak, just above threshold.

V. COMPARISON WITH EXPERIMENTS

Experimental measurements have recently been made of the relative photodetachment cross section for H⁻ in an electric field.¹ More precisely, an 800-MeV beam of H⁻ was passed through a magnetic field, and in the rest frame of the H⁻, that magnetic field is equivalent to an electric field. An yttrium aluminum garnet (YAG) laser beam ($E_p^0=1.1648$ eV in the laboratory) intersected the H⁻ beam at a variable angle, so that the Doppler effect allowed variation of the photon energy in the H⁻ rest frame. In the particular experimental configuration that was used, the laser beam was collinear with the magnetic field. Therefore as this axis was rotated, holding the

magnetic field strength fixed, the effective photon energy and the effective electric field strength varied simultaneously.

If θ is the angle between the beam direction and the laser-and-magnetic-field direction, then the electric field in the rest-frame of H^- is⁸

$$F = \gamma\beta cB \sin\theta \quad (32)$$

and the photon energy in the rest frame of H^- is⁸

$$E_p = E_p^0 \gamma (1 - \beta \cos\theta) . \quad (33)$$

Photodetachment cross sections with π polarization at two different magnetic fields are shown in Fig. 3. The dots represent the experimental data¹ and the solid lines are from the present theory. Since experimental data were not absolute, they were normalized to theoretical

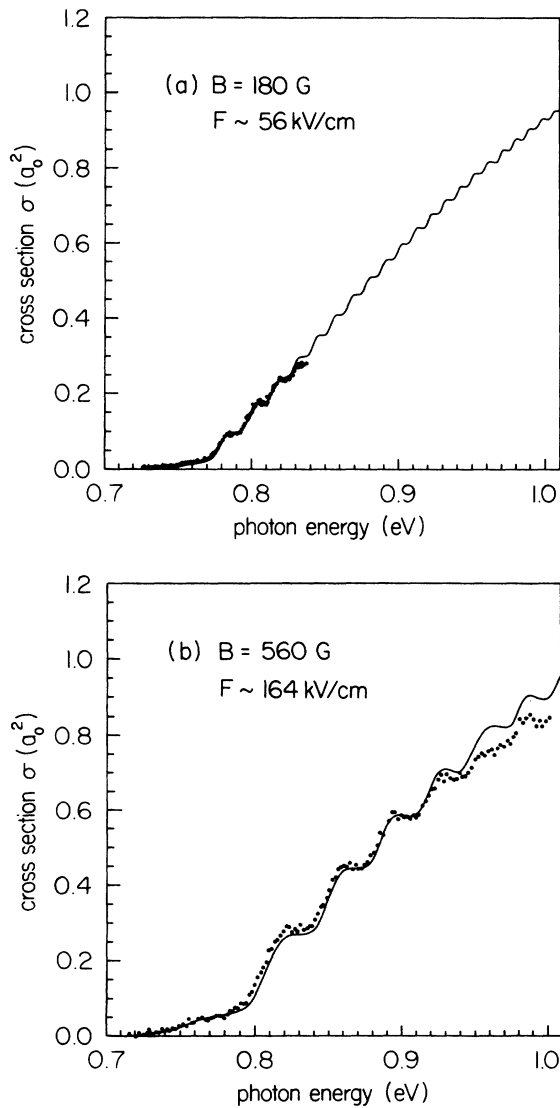


FIG. 3. Near-threshold photodetachment cross section compared with experimental results. (a) F close to 56 kV/cm, (b) F close to 164 keV/cm. Dots are experiment (Ref. 1); solid line is theory.

values at one point. The theoretical predictions are computed from Eq. (16), where D is computed by combining Table I, and Eqs. (20) and (25). Actually the predictions from the much simpler Eq. (30) are indistinguishable from the solid lines in Fig. 3 for photon energy exceeding 0.75 eV. The agreement between this theory and the experimental results is very good.

VI. RELATIONSHIP TO OTHER PHENOMENA

Oscillations are also seen in photoionization of atoms in external magnetic fields, and in other papers we have given a quantitative theory of those oscillations.⁹ The present theory of photodetachment from negative ions in electric fields is very similar to the theory developed in Ref. 9.

In both cases, the final states can be described using a semiclassical approximation, which is accurate everywhere outside the vicinity of the nucleus. Final-state wave functions are therefore correlated with classical trajectories. In both cases, there are trajectories, and associated waves, which propagate out from the vicinity of the initial state, and then are turned back by the external field to return to the vicinity of the initial state (Fig. 4). The superposition of outgoing and returning waves leads to interference, and the resulting oscillations are visible in the absorption spectrum.

In the case of photoionization in a magnetic field, the returning waves were originally thought to be correlated with periodic orbits in the system. We claimed⁹ that *closed* orbits (of which periodic orbits are a subset) lead to measurable oscillations, and this claim has led to much discussion. The present case illustrates this point more clearly. As shown in Fig. 4, none of the orbits associated with the final state are periodic. However, there is one closed orbit in which the electron travels up the potential-energy hill on the z axis, then comes back down to pass through the atomic core again before propagating away downhill. It is that closed but nonperiodic orbit that is responsible for the oscillations shown in Figs. 2 and 3.

Photoionization in electric fields also leads to oscillatory cross sections. The observed phenomena have been successfully described by frame-transformation theory.¹⁰ In future work we plan to examine this phenomenon using the type of semiclassical closed-orbit theory that is used in this paper and in Ref. 9. The primary technical

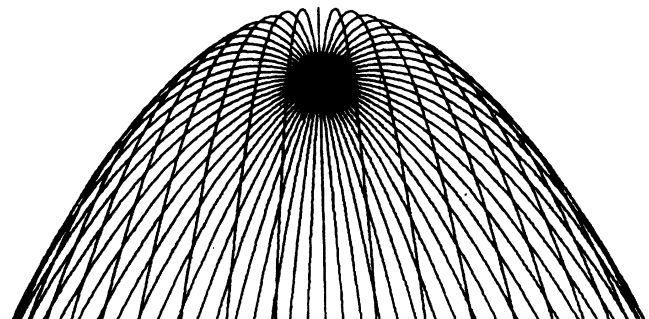


FIG. 4. Trajectories of the outgoing electron in a constant electric field directed along the vertical axis.

difference between the two approaches is that frame-transformation theory [as applied in Ref. 10(a)] uses separation of variables in parabolic coordinates, where closed-orbit theory uses a multidimensional semiclassical approximation. Also the two theories describe modulations in cross sections in very different terms. In Ref. 10 modulations are described as a sequence of quasi-bound resonance states, whereas in Ref. 9, we speak of interference among returning waves leading to sinusoidal oscillations in the cross sections. Thus the language and the physical pictures are somewhat different. Nevertheless, it seems likely that the two theories will lead to similar results.

VII. SUMMARY

A formula [Eq. (16)] was derived for photodetachment from H^- in a static electric field. The formula contains a function $D(x)$, which can be evaluated using Eq. (20) for $x \leq -4.75$, Eq. (25) for $x \geq 4.0$, and Table I for intermediate values of x . The formula provides a quantitative description of tunneling, threshold, and oscillatory effects that have been observed in experiments. The much simpler formula (30) gives a good description of the cross section above threshold.

ACKNOWLEDGMENTS

This research was partially supported by the National Science Foundation and by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research of the U.S. Department of Energy. We thank Dr. J. E. Stewart for kindly providing the experimental data prior to publication.

APPENDIX: THE "NORMALIZATION" CONSTANT

1. Confusion

Fano and Rau,¹¹ following Ohmura and Ohmura,³ used the wave function (3) to discuss the photodetachment cross section for H^- with no electric field present. The free states are then Bessel functions, and the resulting integral [our Eq. (2a)] is a standard one. However, they seem to have miscopied it, and an additional factor of $\sqrt{2}$ should appear on the right-hand side of their Eq. (7.12). Hence their Eq. (7.13) should be (in their notation)

$$\sigma = \frac{64\pi^2}{3(137)} C^2 \frac{k^3}{(k_B^2 + k^2)^3} \quad (\text{A1})$$

(they give 32 instead of 64). They said, "The normalization constant C can be taken from a very accurate calculation of the complete wave function, or it can be adjusted by fitting the scale of the cross-section spectrum," and they cited Ohmura and Ohmura, but they did not actually give the value. (Their " C " is what we call " B .")

The appropriate value was given by Ohmura and Ohmura.³ The quantity they call " C " differs from our quantity " B " by a factor of $(2\pi)^{1/2}$, but the value they give is correct, and consistent with our Eq. (6). On their graph of the photodetachment cross section versus wave-

length, the vertical axis is mislabeled as $K_v \times 10^{19} \text{ cm}^2$; it should be $K_v \times 10^{17} \text{ cm}^2$. By such relabeling, the graph will agree with their formula, and with independent calculations by Geltman.¹² The graph was reprinted in Ref. 11 without correction.

In evaluating the photodetachment cross-section in the presence of an external electric field, Rau and Wong⁵ carried the factor of 2 error into their Eq. (2). They also evaluated the constant C incorrectly. Their value of C^2 is smaller than the appropriate value by a factor of 2.65. When this is combined with the missing factor of 2 from the evaluation of the dipole integral, their formula predicts cross sections that are too small by a factor of 5.3.

Surprisingly, however, their graph of the cross section is correct. Apparently, Rau and Wong used in their calculations the formula of Ohmura and Ohmura instead of their own formula for the free-field cross section.

2. Evaluation of the constant B

One is tempted to say that B should be chosen such that the wave function ψ_i is normalized:

$$1 = \int |\psi_i|^2 d\tau = 2\pi B^2 / k_b, \quad (\text{A2})$$

$$B^2 = k_b / 2\pi.$$

In fact, this is not appropriate. Bethe and Longmire² gave a better method for the evaluation of B .

They noted that Eq. (3) is an approximation that holds only outside of the effective range of the potential energy, and that

$$1 = \int |\psi_i^{\text{exact}}|^2 d\tau$$

$$= \int |\psi_i^{\text{approx}}|^2 d\tau - \int (|\psi_i^{\text{approx}}|^2 - |\psi_i^{\text{exact}}|^2) d\tau.$$

The last integral is proportional to Schwinger's definition of the effective range,² r_{eff} :

$$r_{\text{eff}} = (2\pi B^2)^{-1} \int (|\psi_i^{\text{approx}}|^2 - |\psi_i^{\text{exact}}|^2) d\tau.$$

Therefore

$$1 = 2\pi B^2 / k_b - 2\pi B^2 r_{\text{eff}}$$

or

$$B^2 = \left[\frac{k_b}{2\pi} \right] \frac{1}{(1 - k_b r_{\text{eff}})}. \quad (\text{A3})$$

Ohmura and Ohmura³ found r_{eff} to be $2.646a_0$, and this leads to $B = 0.31552$. The last factor in (A3), $(1 - k_b r_{\text{eff}})^{-1}$, increases the calculated value of B^2 by a factor of 2.655. Without it, Ohmura and Ohmura would not have obtained an accurate photodetachment cross section. This factor was also incorporated correctly in a paper by Reiss⁴ on above-threshold detachment.

Rau and Wong⁵ make a very confusing statement that "only one constant is needed to calculate the photodetachment cross-section." They refer to k_b . Actually both k_b and the effective range r_{eff} are needed, as the factor of 2.65 is a nontrivial correction.

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