Quantum-mechanical calculation of the photodetachment of H^- in electric and magnetic fields with arbitrary orientation

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We derive general quantum-mechanical formulas for the photodetachment cross section of H^- in electric and magnetic fields with arbitrary orientation. The formulas are valid for any linear polarization and for any orientation. We have evaluated the cross-section spectra for different orientations of the electric and magnetic fields and displayed the effects of the orientations upon the oscillatory structures of the cross sections. [S1050-2947(97)11109-X]

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I. INTRODUCTION

The photodetachment of H^- in the presence of electric and magnetic fields has been studied previously both quantum mechanically and closed-orbit theory. Du [1] performed the quantum-mechanical analysis in parallel electric and magnetic fields; Peters, Jaffe, and Delos [2] did the same using closed-orbit theory. Peters and Delos [3] also evaluated the cross section of H^- in perpendicular electric and magnetic fields using both the quantum-mechnical method and closed-orbit theory. For H^- in electric and magnetic fields with any orientation [4], we calculated the cross section by using closed-orbit theory.

In this paper we present a general quantum-mechanical formula for the photodetachment cross section of H^- in electric and magnetic fields with arbitrary orientation. As in earlier treatments [1–3], we assume that the effects of the external fields are so small in the region close to the atomic core that the fields can be neglected, and the binding potential dominates. After the active electron absorbs a photon, it is detached and travels quickly away from the region near the core, entering the region in which the Coulomb interaction with the nucleus can be neglected and the electric and magnetic fields cannot. In the asymptotic region, the Schrödinger equation is separable in Cartesian coordinates. In Sec. II, we present the derivation of the analytic formulas for the photodetachment cross section in electric and magnetic fields with any orientation; in Sec. III, we evaluate and display the cross-section spectra for different orientations of the electric and magnetic fields. Atomic units are used throughout this paper.

II. DERIVATION

A. Initial state

In the region close to the atomic core, we neglect the small effects of the electic and magnetic fields on the active electron of H^-. The initial-state wave function of the active electron is taken as [1–3]

$$\psi_i(\mathbf{r})=B_0\frac{e^{-ik_br}}{r}, \tag{1}$$

where k_b is related to the binding energy of the valence electron by $E_b=k_b^2/2$, and B_0 is a ''scale factor'' with the value being 0.315 52. The momentum representation of the initial wave function is

$$\psi_i(\mathbf{p})=\frac{\sqrt{2/\pi}B_0}{(k_b^2+k^2)}. \tag{2}$$

B. Final states

After being detached by the photon, the active electron propagates quickly away from the region close to the atomic core. Thus, in the final state, we neglect the effects of the short-range binding potential compared to the external fields. The final wave function can be taken to be the wave function of an electron in electric and magnetic fields.

We take the magnetic field $\mathbf{H}_0$ along the positive z axis and take the electric field $\mathbf{F}$ in the x-z plane. The angle between the electric and magnetic fields is denoted by α. It is convenient to separate the electric field $\mathbf{F}$ into two components: one is F_1 ($F_1=F\sin\alpha$) in the positive x direction, and the other is F_2 ($F_2=F\cos\alpha$) in the positive z direction. The Hamiltonian is then given by

$$H=\frac{1}{2}\left[\mathbf{p}-\frac{\mathbf{A}}{c}\right]^2+F_1x+F_2z, \tag{3}$$

where $-F_1x-F_2z$ is the scalar potential of the electric field, and $\mathbf{A}$ is the vector potential of the magnetic field, which is defined by

$$\mathbf{A}=H_0x\hat{\mathbf{j}}, \tag{4}$$

where $\hat{\mathbf{j}}$ is a unit vector directed along the positive y axis. Defining the quantities [3]

$$\varepsilon=\frac{1}{2}p_x^2+\frac{1}{2}\omega_c^2\left[x+\frac{1}{\omega_c}\left(p_y+\frac{F_1}{\omega_c}\right)\right]^2 \tag{5}$$

and

$$H_z=\frac{1}{2}p_z^2+F_2z. \tag{6}$$

The Hamiltonian can be reexpressed by

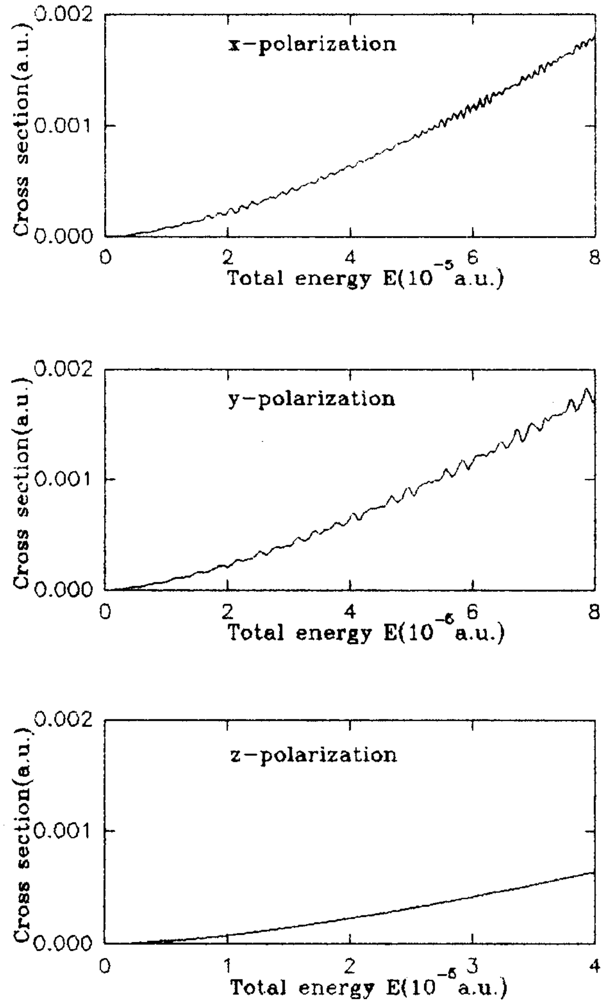

FIG. 1. Photodetachment cross sections of H^- in perpendicular electric and magnetic fields. They are evaluated from the quantum-mechanical formula, Eq. (37), in Ref. [3].

$$H=\varepsilon-\frac{F_1}{\omega_c}p_y-\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2+H_z, \quad (7)$$

where the cyclotron frequency ω_c is equal to H_0/c. It is easy to prove that ε, p_y, and H_z are independently conserved. With the eigenvalues of ε, p_y, and H_z denoted by ε_n, p_{y_0}, and E_{z_0}, and with the wave functions of ε, p_y, and H_z denoted by $\psi_n(x)$, $\psi_y(y)$, and $\psi_z(z)$, we obtain

$$\varepsilon\psi_n(x)=\varepsilon_n\psi_n(x), \quad (8)$$

$$p_y\psi_y(y)=p_{y_0}\psi_y(y), \quad (9)$$

$$H_z\psi_z(z)=E_{z_0}\psi_z(z). \quad (10)$$

Equation (8) is the equation for a harmonic oscillator centered at

$$x_c(p_{y_0})=-\frac{1}{\omega_c}\left[p_{y_0}+\frac{F_1}{\omega_c}\right]. \quad (11)$$

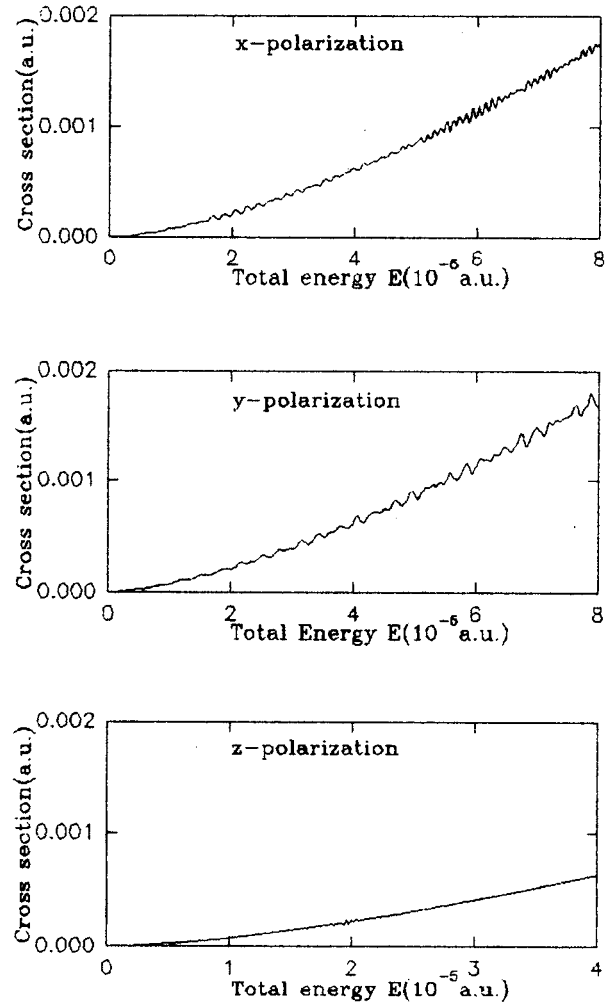

FIG. 2. Photodetachment cross sections of H^- in electric and magnetic fields with the angle of fields being 85°.

The center of the harmonic oscillator depends upon the initial y component p_{y_0} of momentum. If we define the dimensionless quantity

$$X(x,p_{y_0})=\sqrt{\omega_c}[x-x_c], \quad (12)$$

the solution of Eq. (8) is the Hermite function

$$\psi_n(x)=U_n(X(x,p_{y_0})), \quad (13)$$

where the Hermite function is

$$U_n(X)=\left[\left(\frac{\omega_c}{\pi}\right)^{1/2}\frac{1}{2^n n!}\right]^{1/2}\exp(-X^2/2)H_n(X), \quad (14)$$

with $H_n(X)$ being the Hermite polynomial. The eigenvalues of Eq. (8) are

$$\varepsilon_n=(n+1/2)\omega_c \quad (n=0,1,2,\ldots). \quad (15)$$

The solution of Eq. (9) is

$$\psi_y(y)=\frac{1}{\sqrt{2\pi}}e^{ip_{y_0}y}. \tag{16}$$

Defining the dimensionless quantity

$$\xi=(2F_2)^{1/3}\left(\frac{E_{z_0}}{F_2}-z\right), \tag{17}$$

we can write the solution of Eq. (10) as

$$\psi_z(z)=\left[\frac{4}{F_2}\right]^{1/6}\mathrm{Ai}\left[(2F_2)^{1/3}\left(z-\frac{E_{z_0}}{F_2}\right)\right], \tag{18}$$

where Ai is the standard Airy function [7] and $(4/F_2)^{1/6}$ is the ''energy normalized'' constant. With the help of Eqs. (13), (16), and (18), we achieve the final-state wave function and the total energy of the final state

$$\psi_f(\mathbf{r})=\psi_n(x)\psi_y(y)\psi_z(z)$$
$$=U_n(X)\frac{1}{\sqrt{2\pi}}e^{ip_{y_0}y}\left[\frac{4}{F_2}\right]^{1/6}\mathrm{Ai}\left[(2F_2)^{1/3}\left(z-\frac{E_{z_0}}{F_2}\right)\right] \tag{19}$$

and

$$E_f=\varepsilon_n-\frac{F_1}{\omega_c}p_{y_0}-\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2+E_{z_0}. \tag{20}$$

C. An approximation for the final state

In the region close to the atomic core, the small effects of the external fields can be neglected, and then the final state can be taken to be a free state with suitably chosen amplitudes. Therefore, in this region $\psi_n(x)$ can be approximately written as [3]

$$\psi_n(x)\approx\Phi_n(x)=A_n\cos(p_{x_0}x)+B_n\sin(p_{x_0}x), \tag{21}$$

where p_{x_0} is the x component of momentum at $x=0$. A_n and B_n can be determined by the conditions that the approximate wave function, Eq. (21), and its derivative match the exact wave function, Eq. (13), and its derivative at the origin

$$A_n=U_n(X_c),$$

$$B_n=\frac{\sqrt{\omega_c}}{p_{x_0}}U_n'(X_c). \tag{22}$$

The prime in Eq. (22) refers to the differentiation of the Hermite function with respect to X_c, and X_c is

$$X_c=-\sqrt{\omega_c}x_c. \tag{23}$$

The approximate final wave function is then given by

$$\psi_f(\mathbf{r})\cong\Phi_n(x)\frac{1}{\sqrt{2\pi}}e^{ip_{y_0}y}\left[\frac{4}{F_2}\right]^{1/6}\mathrm{Ai}\left[(2F_2)^{1/3}\left(z-\frac{E_{z_0}}{F_2}\right)\right]. \tag{24}$$

D. Transformation to the momentum representation

In momentum space, Eq. (10) becomes

$$\left[\frac{p_z^2}{2}+iF_2\frac{\partial}{\partial p_z}\right]\tilde{\psi}_z(p_z)=E_{z_0}\tilde{\psi}_z(p_z). \tag{25}$$

The solution of Eq. (25), i.e., the momentum representation of Eq. (18) can be given by

$$\tilde{\psi}_z(p_z)=\frac{1}{\sqrt{2\pi F_2}}\exp\left[\frac{i}{F_2}\left(\frac{p_z^3}{6}-E_{z_0}p_z\right)\right]. \tag{26}$$

Finally, transforming to the momentum representation, we obtain the momentum representation of the final-state wave function

$$\tilde{\psi}_f(\mathbf{p})\cong\frac{1}{2\sqrt{F_2}}[(A_n-iB_n)\delta(p_x-p_{x_0})+(A_n+iB_n)$$
$$\times\delta(p_x+p_{x_0})]\delta(p_y-p_{y_0})\exp\left[\frac{i}{F_2}\left(\frac{p_z^3}{6}-E_{z_0}p_z\right)\right]. \tag{27}$$

E. Dipole matrix elements

The dipole matrix element for an arbitrary linear polarization is given by

$$\langle\psi_f|\mathbf{r}|\psi_i\rangle=\langle\tilde{\psi}_f|i\nabla_{\mathbf{p}}|\tilde{\psi}_i\rangle. \tag{28}$$

Substituting Eqs. (2) and (27) into Eq. (28) and integrating Eq. (28), we obtain the dipole matrix element for the linear polarization along the x axis,

$$\left\langle\tilde{\psi}_f\left|i\frac{d}{dp_x}\right|\tilde{\psi}_i\right\rangle$$

$$=-2\sqrt{\frac{2}{\pi F_2}}B_0B_n\int_{-\infty}^{+\infty}\frac{p_{x_0}}{(k_b^2+p_{x_0}^2+p_{y_0}^2+p_z^2)^2}$$
$$\times\exp\left[\frac{i}{F_2}\left(\frac{p_z^3}{6}-E_{z_0}p_z\right)\right]dp_z. \tag{29}$$

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

$$\frac{p_z^2}{2}-E_{z_0}=0. \tag{30}$$

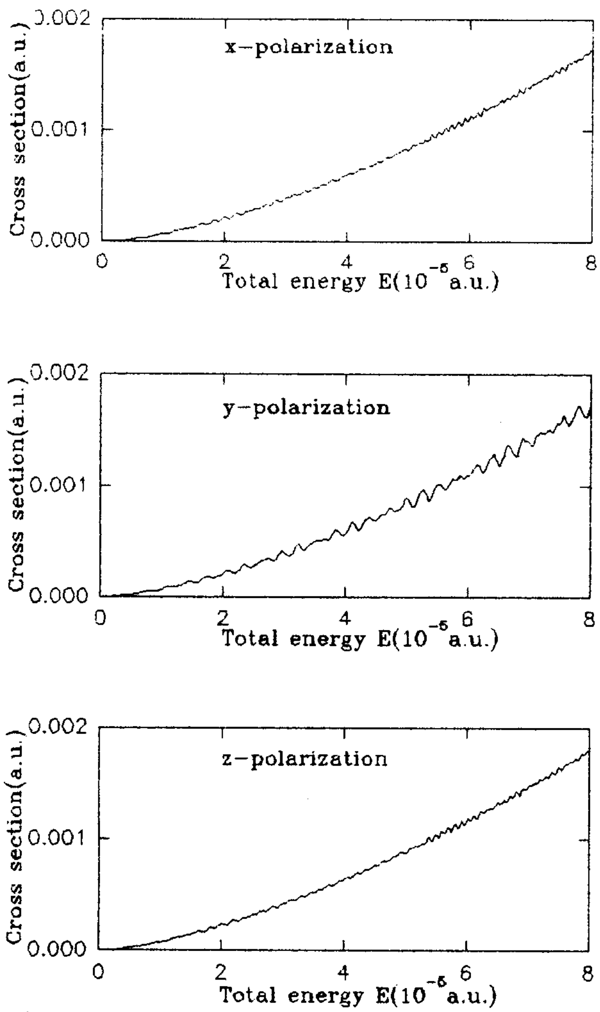

FIG. 3. Photodetachment cross sections of H^- in electric and magnetic fields with the angle of fields being 45°.

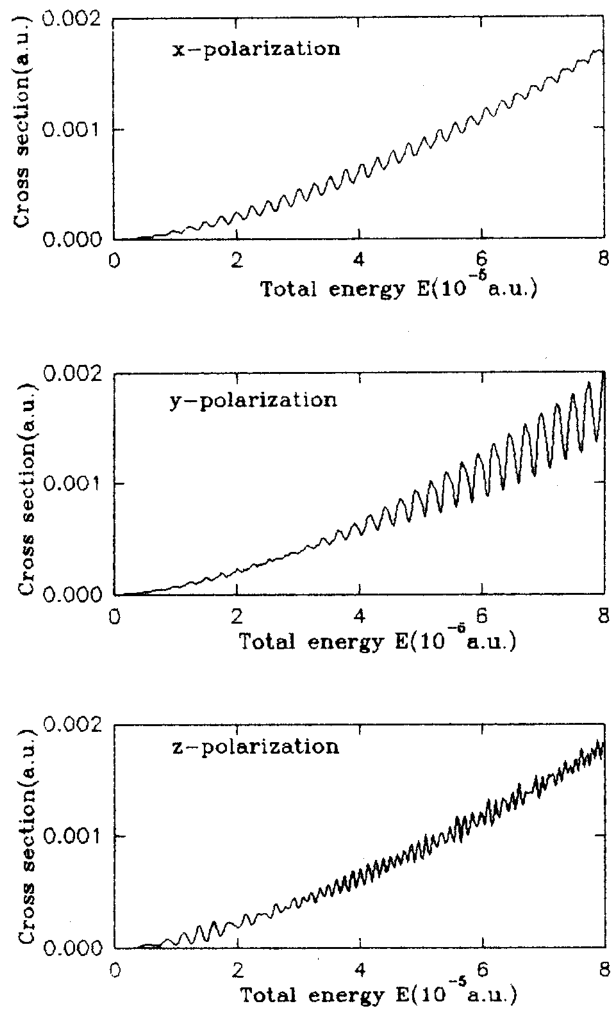

FIG. 4. Photodetachment cross sections of H^- in electric and magnetic fields with the angle of fields being 5°.

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

$$\left\langle \widetilde{\psi}_f \left| i\frac{d}{dp_x} \right| \widetilde{\psi}_i \right\rangle = -2\sqrt{\frac{2}{\pi F_2}} B_0 B_n \frac{p_{x_0}}{(k_b^2+p^2)^2} \times \int_{-\infty}^{+\infty} \exp\left[\frac{i}{F_2}\left(\frac{p_z^3}{6} - E_{z_0} p_z \right) \right] dp_z$$
$$= -\frac{2^{17/6}\pi^{1/2}}{F_2^{1/6}} B_0 B_n \frac{p_{x_0}}{(k_b^2+p^2)^2} \mathrm{Ai} \times \left[-\frac{2E_{z_0}}{(2F_2)^{2/3}} \right]. \tag{31}$$

Following a similar process, we obtain the dipole matrix elements for the other linear polarizations along the y and z axis, respectively,

$$\left\langle \widetilde{\psi}_f \left| i\frac{d}{dp_y} \right| \widetilde{\psi}_i \right\rangle = -i\frac{2^{17/6}\pi^{1/2}}{F_2^{1/6}} B_0 A_n \frac{p_{y_0}}{(k_b^2+p^2)^2} \mathrm{Ai} \times \left[-\frac{2E_{z_0}}{(2F_2)^{2/3}} \right] \tag{32}$$

and

$$\left\langle \widetilde{\psi}_f \left| i\frac{d}{dp_z} \right| \widetilde{\psi}_i \right\rangle = 2^{19/6}\pi^{1/2} F_2^{1/6} B_0 A_n \frac{1}{(k_b^2+p^2)^2} \mathrm{Ai}' \times \left[-\frac{2E_{z_0}}{(2F_2)^{2/3}} \right]. \tag{33}$$

F. Photodetachment cross section

The cross section σ_q for any linear polarization is related to the dipole matrix element by

$$\sigma_q=\frac{2\pi^2}{c}\sum_{n=0}^{+\infty}\int_{-\infty}^{+\infty}dp_{y_0}\times\int_0^{+\infty}dE_{z_0}2E_p|\langle\tilde{\psi}_f|i\nabla_{\mathbf{p}}|\tilde{\psi}_i\rangle|^2\delta(E_f-E),\quad(34)$$

where q represents either x, y, or z. E_p is the energy of the photon, which is equal to the sum of the binding energy E_b and the final energy E of the electron

$$E_p=E_b+E=(k_b^2+k_0^2)/2.\quad(35)$$

Substituting the dipole matrix elements into Eq. (34), we obtain

$$\sigma_x=\sigma_0\frac{3\pi\omega_c}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{-\infty}^{+\infty}dp_{y_0}\int_0^{+\infty}dE_{z_0}\mathrm{Ai}^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n'^2(X_c)\,\delta(E_f-E),\quad(36)$$

where σ_0 is the cross section in the absence of the fields

$$\sigma_0=\frac{64\pi^2B_0^2}{3c}\frac{k_0^3}{(k_b^2+k_0^2)^3}.\quad(37)$$

The two other cross sections for y and z linear polarizations can be obtained in a similar manner,

$$\sigma_x=\sigma_0\frac{3\pi}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{-\infty}^{+\infty}dp_{y_0}\int_0^{+\infty}dE_{z_0}p_{y_0}^2\mathrm{Ai}^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n^2(X_c)\,\delta(E_f-E)\quad(38)$$

and

$$\sigma_x=\sigma_0\frac{3\pi}{k_0^3}(16F_2)^{1/3}\sum_{n=0}^{+\infty}\int_{-\infty}^{+\infty}dp_{y_0}\int_0^{+\infty}dE_{z_0}\mathrm{Ai}^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n^2(X_c)\,\delta(E_f-E).\quad(39)$$

Now let us reduce the cross-section formulas into computational forms. According to the energy conservation, we have

$$E=E_f=\varepsilon_n-\frac{F_1}{\omega_c}p_{y_0}-\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2+E_{z_0},\quad(40)$$

where E_{z_0} is equal to $p_{z_0}/2$, with p_{z_0} being the z component of momentum at the origin. Since E_{z_0} is greater than or equal to zero, the energy conservation equation (40) forces a lower limit on the value of p_{y_0}

$$p_{y_0}\geqslant p_{y_0}^{min}\equiv\frac{\omega_c}{F_1}\left[\varepsilon_n-E-\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2\right].\quad(41)$$

Thus, the integral $\int_{-\infty}^{+\infty}dp_{y_0}$ becomes $\int_{p_{y_0}^{min}}^{+\infty}dp_{y_0}$. Considering the δ function and integrating first over E_{z_0}, we obtain

$$\sigma_x=\sigma_0\frac{3\pi\omega_c}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{p_{y_0}^{min}}^{+\infty}dp_{y_0}\mathrm{Ai}^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n'^2(X_c),\quad(42)$$

$$\sigma_y=\sigma_0\frac{3\pi}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{p_{y_0}^{min}}^{+\infty}dp_{y_0}p_{y_0}{}^2\mathrm{Ai}^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n^2(X_c),\quad(43)$$

and

$$\sigma_z=\sigma_0\frac{3\pi}{k_0^3}(16F_2)^{1/3}\sum_{n=0}^{+\infty}\int_{p_{y_0}^{min}}^{+\infty}dp_{y_0}\mathrm{Ai}'^2\times\left[-\frac{2E_{z_0}}{(2F_2)^{2/3}}\right]U_n^2(X_c),\quad(44)$$

where E_{z_0} is determined by the energy conservation

$$E_{z_0}=E+\frac{F_1}{\omega_c}p_{y_0}+\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2-\varepsilon_n.\quad(45)$$

According to Eqs. (11) and (23), p_{y_0} is related to X_c by the relationship $X_c=[p_{y_0}+F_1/\omega_c]/\sqrt{\omega_c}$, so there is also a minimum value of X_c,

$$X_c\geqslant X_c^{min}\equiv\frac{\sqrt{\omega_c}}{F_1}\left[\varepsilon_n-E+\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2\right].\quad(46)$$

Making a change of variable from p_{y_0} to X_c, the integral $\int_{p_{y_0}^{min}}^{+\infty}dp_{y_0}$ can be changed into $\int_{X_c^{min}}^{+\infty}\sqrt{\omega_c}dX_c$, and E_{z_0} can be reexpressed in the following way:

$$E_{z_0}=\frac{F_1}{\sqrt{\omega_c}}[X_c-X_c^{min}].\quad(47)$$

Finally, we obtain the computational forms of the cross sections

$$\sigma_x=\sigma_0\frac{3\pi\omega_c^{3/2}}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{min}}^{+\infty}dX_c\text{Ai}^2\times\left[-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{min})\right]U_n'^2(X_c), \qquad (48)$$

$$\sigma_y=\sigma_0\frac{3\pi\omega_c^{3/2}}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{min}}^{+\infty}dX_c\left[X_c-\frac{F_1}{\omega_c^{3/2}}\right]^2\text{Ai}^2\times\left[-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{min})\right]U_n^2(X_c), \qquad (49)$$

and

$$\sigma_z=\sigma_0\frac{3\pi\omega_c^{1/2}}{k_0^3}(16F_2)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{min}}^{+\infty}dX_c\text{Ai}'^2\times\left[-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{min})\right]U_n^2(X_c). \qquad (50)$$

III. RESULTS AND DISCUSSION

The range of the energy E is taken to be from 0 to 8.0×10^{-5} a.u. The electric and magnetic fields are chosen to be 18 V/cm and 3/5 T, respectively. Assuming that the light is linearly polarized and using the reduced computational forms, we have evaluated the cross sections for different angles between the fields. Figures 1–5 display the cross-section spectra. We see that the spectra are smooth, rising functions (cross section σ_0 in the absence of fields), superposed upon which are oscillations. There are no divergences on the curves.

As the angle α is close to $\pi/2$, for example, at $\alpha=85°$ (Fig. 1), the amplitudes of the oscillations on the cross section σ_z (Fig. 2) are so small that they are almost invisible. However, the amplitudes of the oscillatory structures upon the cross-section spectra σ_x and σ_y are large. Comparing Fig. 1 to Fig. 2, we can see that cross sections σ_x and σ_y have the same oscillatory structures as the ones at $\alpha=\pi/2$.

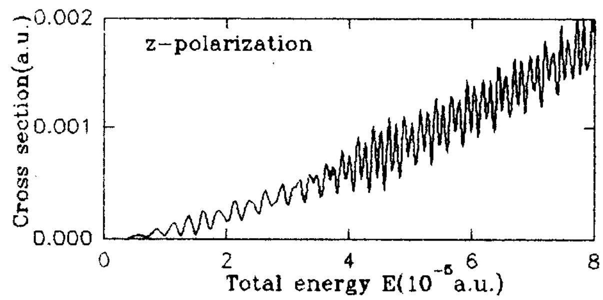

FIG. 5. Photodetachment cross sections of H^- in electric and magnetic fields. The cross section in parallel electric and magnetic fields ($\alpha=0$) is calculated from the quantum-mechanical formula, Eq. (12b), in Ref. [1].

As the value of the angle α decreases from $\pi/2$, the oscillatory amplitudes of σ_z increase quickly. For example, at $\alpha=45°$, the oscillatory amplitudes of σ_z are large and then can be identified clearly. We can see that at this angle, σ_x and σ_z almost have the same oscillatory structures, and the oscillatory structures of σ_x and σ_y are still similar to the ones at $\alpha=\pi/2$. These results are consistent with the predictions of the closed-orbit theory [4].

As the value of the angle α continues to decrease, the oscillatory amplitudes of σ_z continue to increase, and the oscillatory structures of σ_x, σ_y, and σ_z deviate from the ones of $\alpha=\pi/2$. For example, at $\alpha=5°$, we can see this clearly from Fig. 4. Comparing Fig. 4 to Fig. 5, we can see that when the value of α is close to zero, the oscillating structures of cross-section spectra will be tending toward the ones at $\alpha=0$.

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