Analyzing the photodetachment cross section of H^- in electric and magnetic fields with arbitrary orientation

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We present the general quantum-mechanical formula for the photodetachment cross section of H^- in the electric and magnetic fields with any orientation and the comparison of the quantum-mechanical cross sections to the cross sections calculated from the closed-orbit theory. [S1050-2947(97)07006-6]

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The photodetachment of H^- in the presence of electric and magnetic fields has been studied intensively both theoretically and experimentally. Du [1] performed the quantum-mechanical analysis in parallel electric and magnetic fields considering the light polarized along the fields; Peters, Jaffe, and Delos [2] did this by using closed-orbit theory. For H^- in perpendicular electric and magnetic fields, Fabrikant [3] gave the first quantum-mechanical analysis considering light polarized along the electric field; Peters and Delos [4] presented the analysis by using both the quantum-mechanical method and closed-orbit theory. For H^- in the electric and magnetic fields with any orientation [5], we calculated the cross section by using closed-orbit theory.

In this paper we present the general quantum-mechanical formula for the photodetachment cross section of H^- in the electric and magnetic fields with arbitrary orientation. As in earlier treatments [1–7], 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 compared with the binding potential. In the initial state H^- may be regarded as a single electron with zero orbital angular momentum moving in a central binding potential [8,9]. The initial wave function is written in the form $\psi_i(\mathbf{r})=B_0\exp(-k_b r)/r$, where r is the distance from the nuclus, k_b is related to the binding energy $E_b(E_b=k_b^2/2)$ of the electron, and B_0 is a normalization constant. After detached by the photon, the electron is carried into a P state in the field-free case, and travels quickly away from the region near the core, entering a region where the binding potential can be neglected and the electric and magnetic fields dominate. In this region, the Schrödinger equation is separable in Cartesian coordinates. 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. For convenience, we separate the electric field 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

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

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

$$\mathbf{A}=H_0x\mathbf{j}, \tag{2}$$

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

$$\varepsilon=\tfrac{1}{2}p_x^2+\tfrac{1}{2}\omega_c^2\left(x+\frac{1}{\omega_c}\left[p_y+\frac{F_1}{\omega_c}\right]\right)^2 \tag{3}$$

and

$$H_z=\tfrac{1}{2}p_z^2+F_2z, \tag{4}$$

the Hamiltonian can be reexpressed by

$$H=\varepsilon-\frac{F_1}{\omega_c}p_y-\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2+H_z, \tag{5}$$

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. Therefore, we can obtain the final-state function easily, and then calculate the photodetachment cross section for any linear polarisation directly [11]. The photodetachment cross sections for x, y, and z polarizations are given in the following ways, respectively:

$$\sigma_x=\sigma_0\frac{3\pi\omega_c^{3/2}}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{\min}}^{+\infty}dX_cAi^2\times\left(-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{\min})\right)U_n'^2(X_c), \tag{6}$$

$$\sigma_y=\sigma_0\frac{3\pi\omega_c^{3/2}}{k_0^3}\left(\frac{4}{F_2}\right)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{\min}}^{+\infty}dX_c\left[X_c-\frac{F_1}{\omega_c^{3/2}}\right]^2Ai^2\times\left(-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{\min})\right)U_n^2(X_c) \tag{7}$$

and

$$\sigma_z=\sigma_0\frac{3\pi\omega_c^{1/2}}{k_0^3}(16F_2)^{1/3}\sum_{n=0}^{+\infty}\int_{X_c^{\min}}^{+\infty}dX_cAi'^2\times\left(-\frac{2F_1/\sqrt{\omega_c}}{(2F_2)^{2/3}}(X_c-X_c^{\min})\right)U_n^2(X_c), \tag{8}$$

where k_0 is related to the energy E of the electron ($E=k_0^2/2$); X_c and its minimum value $X_c^{\min}$ are related to the y component of momentum at the origin and its minimum value, respectively:

$$X_c=\frac{1}{\sqrt{\omega_c}}\left[p_{y0}+\frac{F_1}{\omega_c}\right], \tag{9}$$

$$X_c^{\min}=\frac{\sqrt{\omega_c}}{F_1}\left[\left(n+\frac{1}{2}\right)\omega_c-E+\frac{1}{2}\left(\frac{F_1}{\omega_c}\right)^2\right]. \tag{10}$$

Ai is the standard Airy function [10] with the prime in it referring to the differentiation of the Airy function Ai(ξ) with respect to ξ; U_n is the Hermite function [10] with the prime in it referring to the differentiation of the Hermite function with respect to X_c; σ_0 is the cross section in the abscence of fields,

$$\sigma_0=\frac{64\pi^2B_0^2}{3c}\frac{k_0^3}{(k_b^2+k_0^2)^3}. \tag{11}$$

The cross sections Eqs. (6)–(8) are valid for any orientation of the fields. As α approaches $\pi/2$ (or 0), they tend to be the ones at $\alpha=\pi/2$ (or $\alpha=0$). As the angle α is close to $\pi/2$, i.e., $F_2\to 0$, the quantity $(2F_1/\sqrt{\omega_c})/(2F_2)^{2/3}$ will become very large. The exact Airy function can then be replaced by its asymptotic expression [10], and Eqs. (6)–(8) can be reduced to the results obtained by Peters and Delos in perpendicular electric and magnetic fields [4]. As the angle α is close to 0, i.e., $F_1\to 0$, the quantity $(2F_1/\sqrt{\omega_c})/(2F_2)^{2/3}$ will become very small. The exact Airy function are almost constant in the interesting range of X_c. Therefore, as $\alpha\to 0$, the Airy function can be taken out of the integral, and Eq. (8) can then be reduced to the cross section σ_z in parallel electric and magnetic fields given by Du [1].

In the following, taking the range of the energy E to be from 0 to 8.0×10^{-5} a.u., and taking the electric and magnetic fields to be 18 V/cm and $\frac{3}{5}$ T, respectively, we evaluate the cross sections for several angles between the fields by using both the quantum mechanical formula Eqs. (6)–(8) and the closed-orbit formula Eq. (46) in Ref. [5]. Figures 1–3 display the cross-section spectra. The spectra are smooth, rising functions (cross section σ_0 in the absence of fields), superposed upon which are oscillations.

For large angle (for example $\alpha=85°$; see Fig. 1), the closed-orbit and quantum-mechanical results have good agreements. At $\alpha=45°$ (Fig. 2), the closed-orbit cross sections for y and z polarizations are basically consistent with the quantum-mechanical results, but the closed-orbit cross section for x polarization deviates obviously from the quantum-mechanical result. As the angle is very small (for example at $\alpha=5°$; see Fig. 3), the closed-orbit cross section σ_z has basic agreement with the quantum-mechanical cross section σ_z, except that the closed-orbit cross section has larger oscillatory amplitudes. For y polarization, the closed-orbit cross section obviously deviates from the quantum-mechanical one, especially at small energies E. For x polarization, the quantum-mechanical cross section has obvious

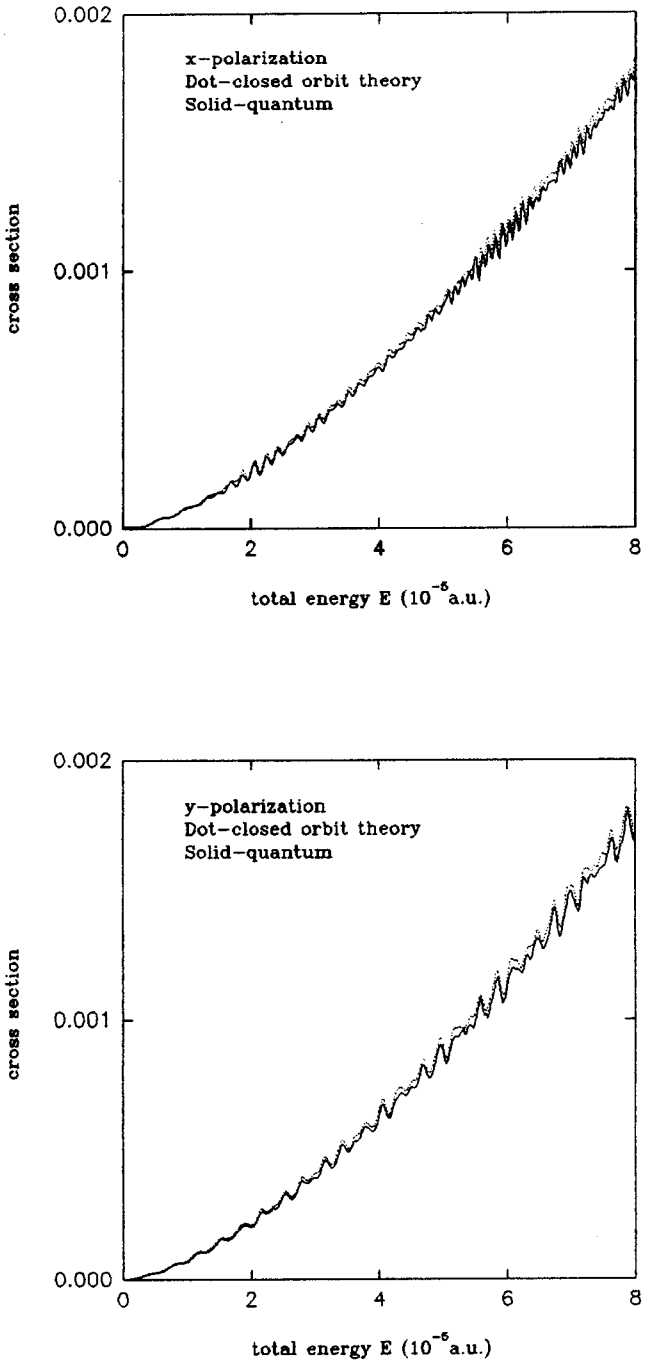

FIG. 1. Photodetachment cross sections (a.u.) of H^- in the electric and magnetic fields with the angle of the fields being 85°. At this angle, the oscillatory structures of both quantum-mechanical and closed-orbit cross sections σ_s are invisible, so they are omitted.

oscillating structures, and the closed-orbit one has no oscillating structures. They are completely different from each other.

According to the above comparison, we see that, for large angles, the closed-orbit results are consistent with the quantum-mechanical results; for small angles, the closed-orbit results deviate greatly from the quantum-mechanical results, except for z polarization. Our preliminary calculations show that the reason for these discrepancies at small angle can be analyzed as follows. In the analysis of photodetachment cross section of H^- with closed-orbit theory [5],

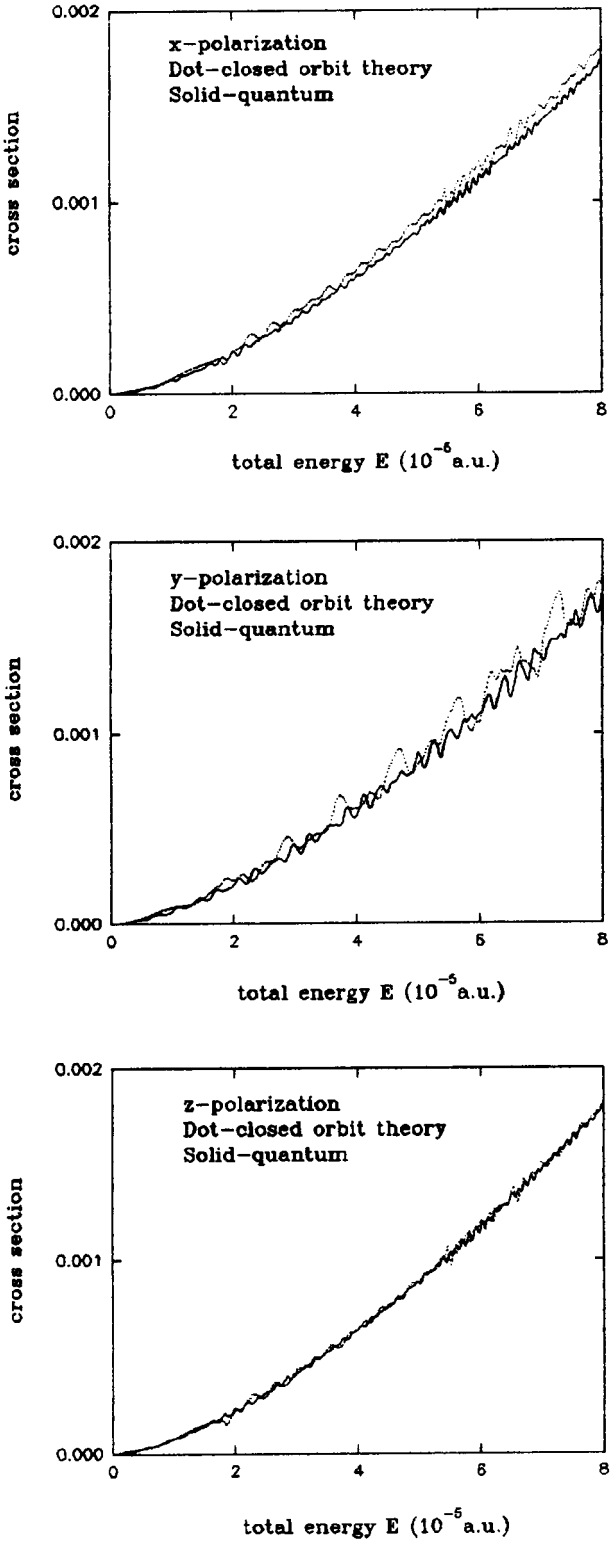

FIG. 2. Photodetachment cross sections (a.u.) of H^- in the electric and magnetic fields with the angle of the fields being 45°.

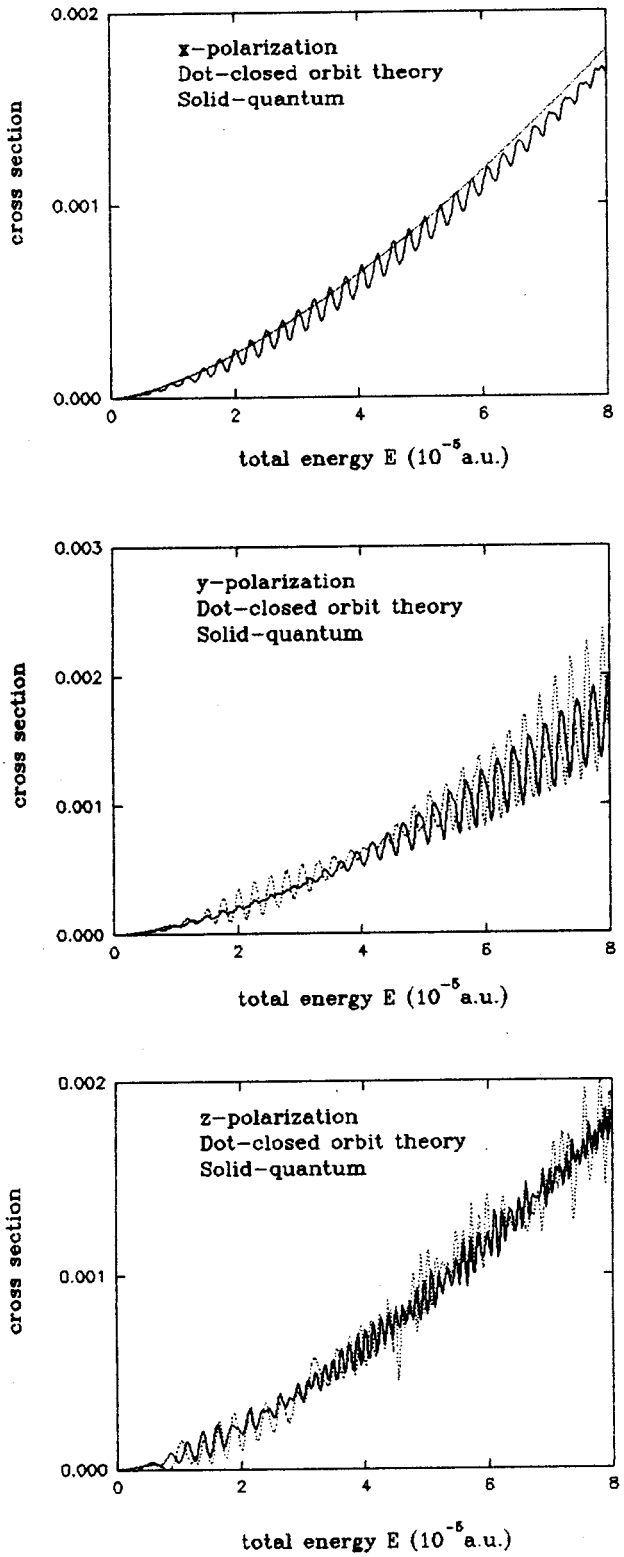

FIG. 3. Photodetachment cross sections (a.u.) of H^- in the electric and magnetic fields with the angle of the fields being 5°.

as in earlier treatments [2,4] we considered only the central closed orbits and families of orbits around them. The central orbits are ones that start from the origin initially, and then return to the origin after some time. However, as the angle is very small, the ''drift'' velocity cF_1/H_0 will become very small. In this case, our preliminary evaluations display that except the central closed orbits and families of orbits around them, there are other trajectories that start from the origin, and then return to the region close to the origin after some time. Although those trajectories do not return to the origin

exactly, they can still overlap with the initial state, and then produce certain effects upon the cross sections. Therefore, as the angle is small, it is not suitable to consider only the central closed orbits and families of orbits around them; the other trajectories that return to the vicinity of the origin should also be included in the calculation of closed-orbitphotodetachment cross sections. A detailed evaluation of this problem is in progress.

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