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Photodetachment cross section of H^- in crossed electric and magnetic fields. II. Quantum formulas and their reduction to the result of the closed-orbit theory

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In this, the second of two papers, we derive general quantum formulas for the photodetachment cross section for H^- in perpendicular electric and magnetic fields. The results are valid for any polarization and can be reduced to the semiclassical results of the first paper [A. D. Peters and J. B. Delos, Phys. Rev. A **47**, 3020 (1993)]: a smooth background plus oscillatory terms. This connection between the quantum and semiclassical results is made using a stationary-phase approximation and it is shown that each stationary-phase point corresponds to a closed orbit.

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I. INTRODUCTION

In this paper, we present a fully-quantum-mechanical formula for the photodetachment cross section for H^- in perpendicular electric and magnetic fields. Fabrikant [1] performed the first analysis considering light polarized along the electric field. Here we extend his results, following a generally similar approach, deriving formulas valid for any polarization. More important, however, we show how these quantum formulas can be reduced to the semiclassical results obtained in the preceding paper.

As in earlier treatments [2], we assume that the field strengths are such that in the "atomic" region, close to the atomic core, the binding potential dominates, and the laboratory fields can be neglected. In this region the initial wave function of the electron, which is in a loosely bound s state, is spherically symmetric and very localized. When the electron absorbs a photon, it quickly propagates out of the atomic region and enters a region where the perpendicular electric and magnetic fields dominate. In this region the Schrödinger equation is separable in Cartesian coordinates.

In Sec. II general quantum formulas are derived. In Sec. III, the general formulas are reduced to forms appropriate for computation. Equation (3.7a) was obtained by Fabrikant, and the formulas for the other cases are closely related. In Sec. IV, we return to the general formulas of Sec. II, and use a stationary-phase approximation to connect the results to the formulas of closed-orbit theory. We will show that each stationary phase point corresponds to a closed orbit.

II. QUANTUM FORMULAS

A. Photodetachment cross section and initial state

The cross section is proportional to the oscillator-strength density $Df(E)$,

$$\sigma=\frac{2\pi^2}{m_e c}e^2\hbar Df(E)\ , \tag{2.1a}$$

where the oscillator-strength density is given by

$$Df(E)=\int df\frac{2m_eE_p}{\hbar^2}|\langle\Psi_f|\mathbf{q}|\Psi_i\rangle|^2\delta(E_f-E)\ . \tag{2.1b}$$

The integral is over all final states of the system, subject to energy conservation implied by the δ function.

We take the initial wave function for the bound electron to be

$$\Psi_i(\mathbf{r})=B_0\frac{e^{-k_br}}{r}\ , \tag{2.2a}$$

where k_b is related to the binding energy of the valence electron by $E_b=(\hbar k_b)^2/2m_e$, and B_0 is a "normalization" constant equal to 0.315 52 in a.u. The Fourier transform of Eq. (2.2a) gives the momentum representation of the initial wave function:

$$\Psi_i(\mathbf{p})=\left[\frac{2}{\hbar^3\pi}\right]^{1/2}B_0\frac{1}{(k_b^2+k^2)}\ . \tag{2.2b}$$

B. "Exact" final state

In the final state, we neglect the binding potential compared to the laboratory fields, and we consider the electron to be moving solely in the electric and magnetic fields. Using the potentials

$$\mathbf{A}_{\text{atomic}}\equiv H_0x\hat{\mathbf{j}}\ ,\qquad \phi_{\text{atomic}}\equiv -Fx\ , \tag{2.3}$$

where $\hat{j}$ refers to a unit vector directed along the y axis, and defining the following quantities:

$$\omega_B\equiv\frac{eF}{m_ec}\ , \tag{2.4a}$$

$$\hat{\varepsilon}\equiv\frac{1}{2m_e}\hat{p}_x^2+\tfrac{1}{2}m_e\omega_B^2(\hat{x}-\hat{x}_c)^2\ , \tag{2.4b}$$

$$\hat{x}_c\equiv-\frac{1}{m_e\omega_B}\left[\hat{p}_y+\frac{eF}{\omega_B}\right]\ , \tag{2.4c}$$

the full Hamiltonian can be written as

$$\hat{H}=\hat{\varepsilon}-\frac{eF}{m_e\omega_B}\hat{p}_y+\frac{1}{2m_e}\hat{p}_z^2-\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2-eV_b\ , \tag{2.5}$$

and we neglect the binding potential V_b. It is easy to show that $\hat{\varepsilon}$, $\hat{p}_y$, and $\hat{p}_z$ all commute with $\hat{H}$ and with each other.

We have decorated the quantum operators with hats. Eigenvalues of these operators are letters without hats (the eigenvalue of $\hat{p}_y$ is p_y or p_{y_0}, and the eigenvalue of $\hat{\varepsilon}$ is ε or ε_n, etc.). There is one exception to this notation. Below, we will use a quantity p_x, which is not an eigenvalue of $\hat{p}_x$ (which, after all, does not commute with H). Instead, p_x is the c number (classical variable) defined such that

$$\varepsilon=\frac{1}{2m_e}p_x^2+\tfrac{1}{2}m_e\omega_B^2(x-x_c)^2\ , \tag{2.6a}$$

$$\varepsilon_n=\frac{1}{2m_e}p_x^{(n)2}+\tfrac{1}{2}m_e\omega_B^2(x-x_c)^2\ , \tag{2.6b}$$

$$E=\frac{1}{2m_e}p_x^2+\tfrac{1}{2}m_e\omega_B^2(x-x_c)^2-\frac{eF}{m_e\omega_B}p_{y_0}+\frac{1}{2m_e}p_{z_0}^2-\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2 . \tag{2.6c}$$

p_x is therefore a function of x (and it depends parametrically on ε and p_{y_0} or E, p_{y_0}, and p_{z_0}). Furthermore, we define the quantity p_{x_0} as the value obtained from Eq. (2.6) when $x=0$. It follows that

$$E=\frac{1}{2m_e}p_{x_0}^2+\frac{1}{2m_e}p_{y_0}^2+\frac{1}{2m_e}p_{z_0}^2\ . \tag{2.7}$$

From Eq. (2.5), the final states Ψ_i are

$$\Psi_f=\Psi_{n,p_{y_0},p_{z_0}}(x,y,z)=X_{n,p_{y_0}}(x)e^{i(p_{y_0}/\hbar)y}e^{i(p_{z_0}/\hbar)z}\ . \tag{2.8}$$

The equation governing $X_{n,p_{y_0}}(x)$ is

$$\hat{\varepsilon}X_{n,p_{y_0}}(x)=\varepsilon_n X_{n,p_{y_0}}(x)\ , \tag{2.9}$$

and this is the equation for a harmonic oscillator centered at

$$x_c=x_c(p_{y_0})=-\frac{1}{m_e\omega_B}\left[p_{y_0}+\frac{eF}{\omega_B}\right]\ . \tag{2.10}$$

Note that the center of the harmonic oscillator depends upon the initial y component of momentum. If we define the dimensionless quantity

$$\chi(x,p_{y_0})\equiv\left[\frac{m_e\omega_B}{\hbar}\right]^{1/2}[x-x_c(p_{y_0})]\ , \tag{2.11a}$$

the solution to the eigenvalue Eq. (2.9) is

$$X_{n,p_{y_0}}(x)=\mathcal{H}_n(\chi(x,p_{y_0}))\ , \tag{2.11b}$$

where the Hermite function is

$$\mathcal{H}_n(\chi)=\left[\left[\frac{m_e\omega_B}{\pi\hbar}\right]^{1/2}\frac{1}{2^n n!}\right]^{1/2}e^{-(1/2)\chi^2}H_n(\chi)\ , \tag{2.12}$$

with $H_n(\chi)$ being the Hermite polynomials. The eigenvalues are the harmonic-oscillator energies

$$\varepsilon_n=\hbar\omega_B(n+\tfrac{1}{2})\ , \tag{2.13}$$

and the total energy of the final state is

$$\begin{aligned}E_f&=E_{n,p_{y_0},p_{z_0}}\\&=\varepsilon_n-\frac{eF}{m_e\omega_B}p_{y_0}+\frac{1}{2m_e}p_{z_0}^2-\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2\\&=\frac{1}{2m_e}p_{x_0}^{(n,p_{y_0})^2}+\frac{1}{2m_e}p_{y_0}^2+\frac{1}{2m_e}p_{z_0}^2\ .\end{aligned} \tag{2.14}$$

C. An approximation for the final state

In the coordinate representation, the initial wave function is very localized. In contrast, the spatial extent of the Hermite function is on the order of the cyclotron radius, i.e., thousands of a_0. We can therefore make a simplified WKB approximation for $X_{n,p_{y_0}}(x)$: over a distance comparable to the size of the atom, we consider the final state to be a free state with suitably chosen amplitude and phase,

$$X_{n,p_{y_0}}(x)\simeq\Phi_n(x,p_{y_0})\equiv A_n(p_{y_0})\cos\left[\frac{p_{x_0}}{\hbar}x\right]+B_n(p_{y_0})\sin\left[\frac{p_{x_0}}{\hbar}x\right]\ . \tag{2.15}$$

The appropriate value of p_{x_0}, which depends on n and p_{y_0}, was defined in Eq. (2.7): it is the classical x component of the momentum at $x=0$.

We evaluate the coefficients by requiring that our approximate wave function (Φ_n) and its derivative match the exact wave function and its derivative at the origin. We require that

$$\begin{aligned}&X_{n,p_{y_0}}(x=0)=\Phi_n(x=0,p_{y_0})\ ,\\&\left[\frac{d}{dx}X_{n,p_{y_0}}(x)\right]_{x=0}=\left[\frac{d}{dx}\Phi_n(x,p_{y_0})\right]_{x=0}\ .\end{aligned} \tag{2.16}$$

With these conditions, we find that

$$\begin{aligned}&A_n(p_{y_0})=\mathcal{H}_n(\chi_c(p_{y_0}))\ ,\\&\frac{p_{x_0}}{\hbar}B_n(p_{y_0})=\left[\frac{m_e\omega_B}{\hbar}\right]^{1/2}\mathcal{H}_n'(\chi_c(p_{y_0}))\ .\end{aligned} \tag{2.17}$$

The prime in Eq. (2.17) refers to differentiation of the Hermite function with respect to $\chi_c(p_{y_0})$, and

$$\chi_c(p_{y_0})=\chi(x=0,p_{y_0})=-\left[\frac{m_e\omega_B}{\hbar}\right]^{1/2} x_c(p_{y_0}) . \quad (2.18)$$

The approximation to the final state is then given by

$$\Psi_f(\mathbf{r})\simeq\Phi_n(x,p_{y_0})\frac{1}{\sqrt{2\pi\hbar}}e^{i(p_{y_0}/\hbar)y}\frac{1}{\sqrt{2\pi\hbar}}e^{i(p_{z_0}/\hbar)z} . \quad (2.19)$$

Transforming to the momentum representation, we obtain

$$\tilde{\Psi}_f(\mathbf{p})\simeq\tilde{\Phi}_n(p_x,p_{y_0})\delta(p_y-p_{y_0})\delta(p_z-p_{z_0}) , \quad (2.20a)$$

where

$$\tilde{\Phi}_n(p_x,p_{y_0})=\sqrt{\hbar\pi/2}[(A_n-iB_n)\delta(p_x-p_{x_0}) + (A_n+iB_n)\delta(p_x+p_{x_0})] . \quad (2.20b)$$

D. Dipole matrix elements

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

$$\langle\Psi_f|\mathbf{q}|\Psi_i\rangle\equiv\langle\tilde{\Psi}_f|i\hbar\nabla_p|\tilde{\Psi}_i\rangle . \quad (2.21)$$

Consider for the moment x-polarized light. Integrating Eq. (2.21) using Eq. (2.20), we obtain

$$\left\langle\tilde{\Psi}_f\left|i\hbar\frac{d}{dp_x}\right|\tilde{\Psi}_i\right\rangle=\int_{-\infty}^{+\infty}\tilde{\Phi}_n(p_x,p_{y_0})i\hbar\frac{d}{dp_x} \times\left[\left[\frac{2}{\hbar^3\pi}\right]^{1/2}B_0\frac{1}{(k_b^2+k^2)}\right]dp_x = \frac{-4B_0}{\hbar^2}\frac{p_{x_0}}{(k_b^2+k_0^2)^2}B_n(p_{y_0}) . \quad (2.22a)$$

The two other polarizations follow in a similar manner:

$$\left\langle\tilde{\Psi}_f\left|i\hbar\frac{d}{dp_y}\right|\tilde{\Psi}_i\right\rangle=\frac{-4iB_0}{\hbar^2}\frac{p_{y_0}}{(k_b^2+k_0^2)^2}A_n(p_{y_0}) , \quad (2.22b)$$

$$\left\langle\tilde{\Psi}_f\left|i\hbar\frac{d}{dp_z}\right|\tilde{\Psi}_i\right\rangle=\frac{-4iB_0}{\hbar^2}\frac{p_{z_0}}{(k_b^2+k_0^2)^2}A_n(p_{y_0}) , \quad (2.22c)$$

and we have used $(\hbar\mathbf{k}_0)\equiv\mathbf{p}_0$.

E. The photodetachment cross section

The cross section for x, y, or z linear polarization in perpendicular electric and magnetic fields is given by the expression

$$\sigma_q=\frac{2\pi^2e^2\hbar}{m_ec}\sum_{n=0}^{\infty}\int_{-\infty}^{+\infty}dp_{y_0}\int_{-\infty}^{+\infty}dp_{z_0}\frac{2m_eE_p}{\hbar^2}|\langle\tilde{\Psi}_f|i\hbar\nabla_p|\tilde{\Psi}_i\rangle|^2\delta(E_f-E) . \quad (2.23)$$

The integral over final states of Eq. (2.1), $\int df$, has become explicit: $\sum_{n=0}^{\infty}\int dp_{y_0}\int dp_{z_0}$. The energy of the photon (E_p) is given by the sum of the energy (E_b) and the final-state energy of the electron (E_f):

$$E_p=E_b+E_f=\frac{1}{2m_e}\hbar^2(k_b^2+k_0^2) . \quad (2.24)$$

Substituting the dipole matrix elements (2.22) into (2.21) and defining the following factors:

$$F_x(n,p_{y_0},p_{z_0})\equiv\tfrac{1}{2}\hbar\omega_B\mathcal{H}_n'^2(\chi_c(p_{y_0})) , \quad (2.25a)$$

$$F_y(n,p_{y_0},p_{z_0})\equiv\frac{1}{2m_e}p_{y_0}^2\mathcal{H}_n^2(\chi_c(p_{y_0})) , \quad (2.25b)$$

$$F_z(n,p_{y_0},p_{z_0})\equiv\frac{1}{2m_e}p_{z_0}^2\mathcal{H}_n^2(\chi_c(p_{y_0})) , \quad (2.25c)$$

the cross section is expressed as

$$\sigma_q=\sigma_0 3\frac{\hbar}{(\hbar k_0)^3}\sum_{n=0}^{\infty}\int dp_{y_0}\int dp_{z_0}F_q(n,p_{y_0},p_{z_0}) \times\delta(E_{n,p_{y_0},p_{z_0}}-E) , \quad (2.25d)$$

where q can be either x, y, or z. The no-field cross section is

$$\sigma_0=\frac{64\pi^2B_0^2}{3c}\frac{k_0^3}{(k_b^2+k_0^2)^3}\frac{e^2}{\hbar} . \quad (2.26)$$

III. REDUCTION OF CROSS-SECTION FORMULAS TO COMPUTATIONAL FORM

We now reduce Eq. (2.25) to a form suitable for computation. We begin by integrating over p_{z_0}, and incorporating the δ function.

The δ function will vanish unless

$$\varepsilon_n-\frac{eF}{m_e\omega_B}p_{y_0}+\frac{1}{2m_e}p_{z_0}^2-\left[E+\frac{1}{2}\frac{eF}{m_e\omega_B^2}\right]=0 , \quad (3.1)$$

which, since p_{z_0} must be real, forces a lower limit to the integral over p_{y_0}. This value is given by

$$p_{y_0}\geq p_{y_0}^{\min}\equiv\frac{m_e\omega_B}{eF}\left[\varepsilon_n-E-\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2\right] \quad (3.2)$$

and

$$\int_{-\infty}^{+\infty} dp_{y_0} \to \int_{p_{y_0}^{\min}}^{+\infty} dp_{y_0} \, .$$

By defining the energy $E_{z_0}=(1/2m_e)p_{z_0}^2$ we can convert the integral over the momentum in the z direction to an integral over the energy E_{z_0}. Since the integrand is a symmetric function of p_{z_0}, there is an extra factor of 2 which appears when the change of variable is made. We find that the cross section can be written as

$$\sigma_q=\sigma_0 3\frac{\hbar}{(\hbar k_0)^3}\sum_{n=0}^{\infty}\int_{p_{y_0}^{\min}}^{\infty} dp_{y_0}\left[\frac{2m_e}{E-\varepsilon_n+\dfrac{eF}{m_e\omega_B}p_{y_0}+\dfrac{1}{2m_e}\left[\dfrac{eF}{\omega_B}\right]^2}\right]^{1/2} \times F_q\left[n,p_{y_0},\left\{2m_e\left[E-\varepsilon_n+\frac{eF}{m_e\omega_B}p_{y_0}+\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2\right]\right\}^{1/2}\right] . \tag{3.3}$$

The final step in the reduction is to make a change of variable to $\chi_c(p_{y_0})$, which was previously defined in Eq. (2.18). From Eq. (3.2) there is a minimum value of χ_c:

$$\chi_c \ge \chi_n^{\min}=\frac{1}{\sqrt{\hbar m_e\omega_B}}\left[p_{y_0}^{\min}+\frac{eF}{\omega_B}\right] =\frac{1}{eF}\left[\frac{m_e\omega_B}{\hbar}\right]^{1/2}\left[\varepsilon_n-E+\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2\right] , \tag{3.4}$$

so

$$\left[E-\varepsilon_n+\frac{eF}{m_e\omega_B}p_{y_0}+\frac{1}{2m_e}\left[\frac{eF}{\omega_B}\right]^2\right] =eF\left[\frac{\hbar}{m_e\omega_B}\right]^{1/2}(\chi_c-\chi_n^{\min}) . \tag{3.5}$$

With this change of variable we find

$$\sigma_q=\sigma_0 3\frac{m_e^{5/4}\omega_B^{7/4}}{k_0^3\sqrt{2eF}\,\hbar^{3/4}}\sum_{n=0}^{\infty}D_q(\chi_n^{\min}) , \tag{3.6}$$

where

$$D_x(\chi_n^{\min})=\int_{\chi_n^{\min}}^{+\infty}\frac{\mathcal{H}_n'^2(\chi_c)}{(\chi_c-\chi_n^{\min})^{1/2}}d\chi_c , \tag{3.7a}$$

$$D_y(\chi_n^{\min})=\int_{\chi_n^{\min}}^{+\infty}\left[\chi_c-\frac{eF}{\sqrt{\hbar m_e\omega_B}}\right]^2 \times\frac{\mathcal{H}_n^2(\chi_c)}{(\chi_c-\chi_n^{\min})^{1/2}}d\chi_c , \tag{3.7b}$$

$$D_z(\chi_n^{\min})=\int_{\chi_n^{\min}}^{+\infty}\frac{2eF}{\omega_B\sqrt{\hbar m_e\omega_B}}(\chi_c-\chi_n^{\min}) \times\frac{\mathcal{H}_n^2(\chi_c)}{(\chi_c-\chi_n^{\min})^{1/2}}d\chi_c . \tag{3.7c}$$

These are the desired computational forms that have been used to evaluate the quantum photodetachment cross section numerically. At this point it is difficult to see any connection between the quantum result and the semiclassical formula obtained in our first paper.

IV. REDUCTION TO THE RESULT OF CLOSED-ORBIT THEORY

A. Expression as a momentum integral

We now reduce the quantum photodetachment cross-section formulas to the smooth background plus oscillatory terms that were obtained from closed-orbit theory. To do this, we return to Eq. (2.25), use a WKB approximation to $\mathcal{H}_n$, and evaluate the integrals using a stationary phase approximation.

In Eq. (2.6) we defined the classical quantity $p_x(x)$ as the momentum classically associated with the position x through the conservation laws. In this section, it is best to think of p_x as a function of x and of E, p_{y_0}, and p_{z_0}, as specified in Eq. (2.6c). This function is used to give the WKB approximation for $X(x)$:

$$X_{n,p_{y_0}}(x)\simeq\pm\left[\frac{2m_e\omega_B}{\pi}\right]^{1/2}\frac{1}{|p_x(x)|^{1/2}} \times\sin\left[\frac{1}{\hbar}\int_{x_{\mathrm{TP}}}^{x}p_x(x')dx'-\frac{\pi}{4}\right] . \tag{4.1}$$

x_{TP} is the larger of the two turning points. The derivative of the above function with respect to x is

$$\frac{d}{dx}X_{n,p_{y_0}}(x)\simeq\pm\left[\frac{2m_e\omega_B}{\pi}\right]^{1/2}\frac{|p_x(x)|^{1/2}}{\hbar} \times\cos\left[\frac{1}{\hbar}\int_{x_{\mathrm{TP}}}^{x}p_x(x')dx'-\frac{\pi}{4}\right] . \tag{4.2}$$

Using the trigonometric identities

$$\cos^2(\eta)=\tfrac{1}{2}+\tfrac{1}{2}\cos(2\eta) , \quad \sin^2(\eta)=\tfrac{1}{2}-\tfrac{1}{2}\cos(2\eta) , \tag{4.3}$$

and the WKB functions listed above, we can evaluate Eq. (2.25) and obtain

$$F_x=\frac{m_e\omega_B}{\pi}\frac{p_{x_0}^2}{2m_e}\frac{1}{p_{x_0}}\left[1-\sin\frac{1}{\hbar}S_x\right], \tag{4.4a}$$

$$F_y=\frac{m_e\omega_B}{\pi}\frac{p_{y_0}^2}{2m_e}\frac{1}{p_{x_0}}\left[1+\sin\frac{1}{\hbar}S_x\right], \tag{4.4b}$$

$$F_z=\frac{m_e\omega_B}{\pi}\frac{p_{z_0}^2}{2m_e}\frac{1}{p_{x_0}}\left[1+\sin\frac{1}{\hbar}S_x\right], \tag{4.4c}$$

where the phase is given by

$$S_x=-2\int_{x_{TP}^{(n,p_y^0)}}^{0}p_x(x')dx' . \tag{4.5}$$

When $F_q(n,p_{y_0},p_{z_0})$ is put into Eq. (3.3), each cross section is the sum of two terms. The first term is a smooth function and comes from the 1 in Eq. (4.4). The second term is oscillatory and arises from the S_x in these same equations. In the next two sections the integrals of the photodetachment cross section are evaluated.

If the energy is large enough, there will be many harmonic-oscillator levels involved in the summation of Eq. (3.6). The density of states will be high and the integrand will vary slowly over Δn. In this case we can make the change $\sum_{n=0}^{\infty}\to(1/\hbar\omega_B)\int_0^{\infty}$. Making the further change of variable from ε to p_{x_0}, where

$$\begin{aligned}p_{x_0}&=\left[2m_e\varepsilon-\left[p_{y_0}+\frac{eF}{\omega_B}\right]^2\right]^{1/2},\\ d\varepsilon&=\frac{1}{m_e}p_{x_0}dp_{x_0},\end{aligned} \tag{4.6}$$

then for symmetric functions of p_{x_0} we can replace the summation with $\sum_{n=0}^{\infty}\to(1/2\hbar m_e\omega_B)\int_{-\infty}^{+\infty}dp_{x_0}p_{x_0}$, and the cross section is

$$\sigma_q=\sigma_0 3\frac{\hbar}{(\hbar k_0)^3}\frac{1}{2\hbar m_e\omega_B}\int_{-\infty}^{+\infty}dp_{x_0}\int_{-\infty}^{+\infty}dp_{y_0}\int_{-\infty}^{+\infty}dp_{z_0}\frac{m_e\omega_B}{\pi}\frac{p_q^2}{2m_e}\left[1\mp\sin\frac{1}{\hbar}S_x\right]\delta\left[\frac{1}{2m_e}p^2-E\right]. \tag{4.7}$$

The sign is minus for x polarization and plus for y or z polarization.

B. The evaluation of the smooth term

The smooth term of Eq. (4.7) is

$$\sigma_q^{\rm smt}=\sigma_0\frac{3}{2\pi}\frac{1}{(\hbar k_0)^3}\int d\mathbf{p}\frac{p_q^2}{2m_e}\delta\left[\frac{1}{2m_e}p^2-E\right]. \tag{4.8}$$

The three integrals (for $q=x$, y, or z) are obviously equal, and each is equal to

$$\sigma_q^{\rm smt}=\sigma_0\tfrac{1}{3}E_f\int d\mathbf{p}\,\delta\left[\frac{1}{2m_e}p^2-E\right]. \tag{4.9}$$

The last integral is related to the area of the energy shell in p space. By going to polar coordinates in momentum space, we find that it is that area times dp/dE:

$$\int d\mathbf{p}\,\delta\left[\frac{p^2}{2m_e}-E\right]=4\pi p_0^2\frac{dp_E}{dE}=4\pi p_0^2\frac{m_e}{p_0}, \tag{4.10}$$

where $p_0=\hbar k_0=(p_{x_0}^2+p_{y_0}^2+p_{z_0}^2)^{1/2}$. Substituting this into Eq. (4.9), the smooth contribution to the photodetachment cross section is the no-field cross section, precisely

$$\sigma_q^{\rm smt}=\sigma_0 . \tag{4.11}$$

C. Reexpression of the oscillatory term

Next we evaluate the oscillatory contribution to the photodetachment cross section. To do this we need to think carefully about the meaning of the function S_x defined in Eq. (4.5). We said that we think of $p_x(x)$ as depending parametrically upon E, p_{y_0}, and p_{z_0} through Eq. (2.6c). Therefore, S_x also depends on these three parameters. Also, through the relationship, Eq. (2.7), that connects p_{x_0} to (E,p_{y_0},p_{z_0}), we can think of S_x as an even function of $(p_{x_0},p_{y_0},p_{z_0})$. This thought is implicit in converting Eq. (2.25) to Eq. (4.7). Now we restrict p_{x_0} to positive values, convert to polar coordinates in momentum space, and integrate over p_0. From Eq. (4.7) we obtain

$$\sigma_q^{\rm osc}=(\mp)\sigma_0\frac{3}{\pi}\frac{1}{(\hbar k_0)^3}\int_0^{+\infty}dp_{x_0}\int_{-\infty}^{+\infty}dp_{y_0}\int_{-\infty}^{+\infty}dp_{z_0}\frac{p_q^2}{2m_e}\sin\frac{1}{\hbar}S_x(p_{x_0},p_{y_0},p_{z_0})\delta\left[\frac{1}{2m_e}p_0^2-E\right] \tag{4.12a}$$

$$=(\mp)\sigma_0\frac{3}{4\pi}\frac{1}{2}\int d\Omega\frac{p_q^2}{p_0^2}\sin\frac{1}{\hbar}S_x(p_0,\Omega), \tag{4.12b}$$

where the angular integral includes the $p_{x_0}>0$ hemisphere.

For further amusement, we can write the argument of the sin in another way. The semiclassical quantization condition associated with the x motion,

$$\oint p_x(x',\mathbf{p}_0)dx'=(n+\tfrac{1}{2})2\pi\hbar, \tag{4.13}$$

can be written as

$$\frac{1}{\hbar}\oint p_x(x',\mathbf{p}_0)dx' - \pi = n2\pi \ . \tag{4.14}$$

With this result we express $\sin(S_x)$ in the following way:

$$\sin\frac{1}{\hbar}S_x = \sin\left[\frac{1}{\hbar}S_{x,K} - K\pi\right] , \tag{4.15}$$

where

$$S_{x,K} = 2\int_0^{x_{\mathrm{TP}}} p_x(x,\mathbf{p}_0)dx' + K\oint p_x(x',\mathbf{p}_0)dx' \ . \tag{4.16}$$

We will seek the stationary phase points of the integral [Eq. (4.12b)].

D. An action function

First let us indulge in an apparent digression. Consider a three-dimensional family of classical trajectories, in which each trajectory has the same energy E, each begins at the origin $x=y=z=0$ propagating in any direction, but with the restriction that the initial x component of momentum p_{x_0} is positive. Let each trajectory run until the first time it returns to $x=0$ (see Fig. 1). Let the action integral for each trajectory with the specified end points be defined as

$$S_0(p_0,\Omega_0) \equiv \int \mathbf{p}\cdot d\mathbf{q}' \ . \tag{4.17}$$

Now let us allow the trajectories to continue through one or more cyclotron periods until they again pass through the surface $x=0$ with $\dot{x}=(1/m_e)p_x<0$. Let the associated action integral be denoted

$$S_K(p_0,\Omega_0) = \int \mathbf{p}\cdot d\mathbf{q}' + K\oint \mathbf{p}\cdot d\mathbf{q}' , \tag{4.18}$$

where the cycle integral refers to one cyclotron period.

Consider the function

$$S_{x,K}(p_0,\Omega_0) = S_K(p_0,\Omega_0) - S_{y,K}(p_0,\Omega_0) - S_{z,K}(p_0,\Omega_0) \ . \tag{4.19}$$

The latter two terms are defined as the y and z parts of the action integral between the given initial and final points,

$$\begin{aligned} S_{y,K} &= \int_0^{y_K} p_y dy = p_{y_0} y_K \ , \\ S_{z,K} &= \int_0^{z_K} p_z dz = p_{z_0} z_K \ , \end{aligned} \tag{4.20}$$

where y_K and z_K are the end points of the trajectory having initial conditions (p_0,Ω_0) after the Kth cycle $(K=0,1,2,\dots)$. We have used the fact that p_y and p_z are conserved.

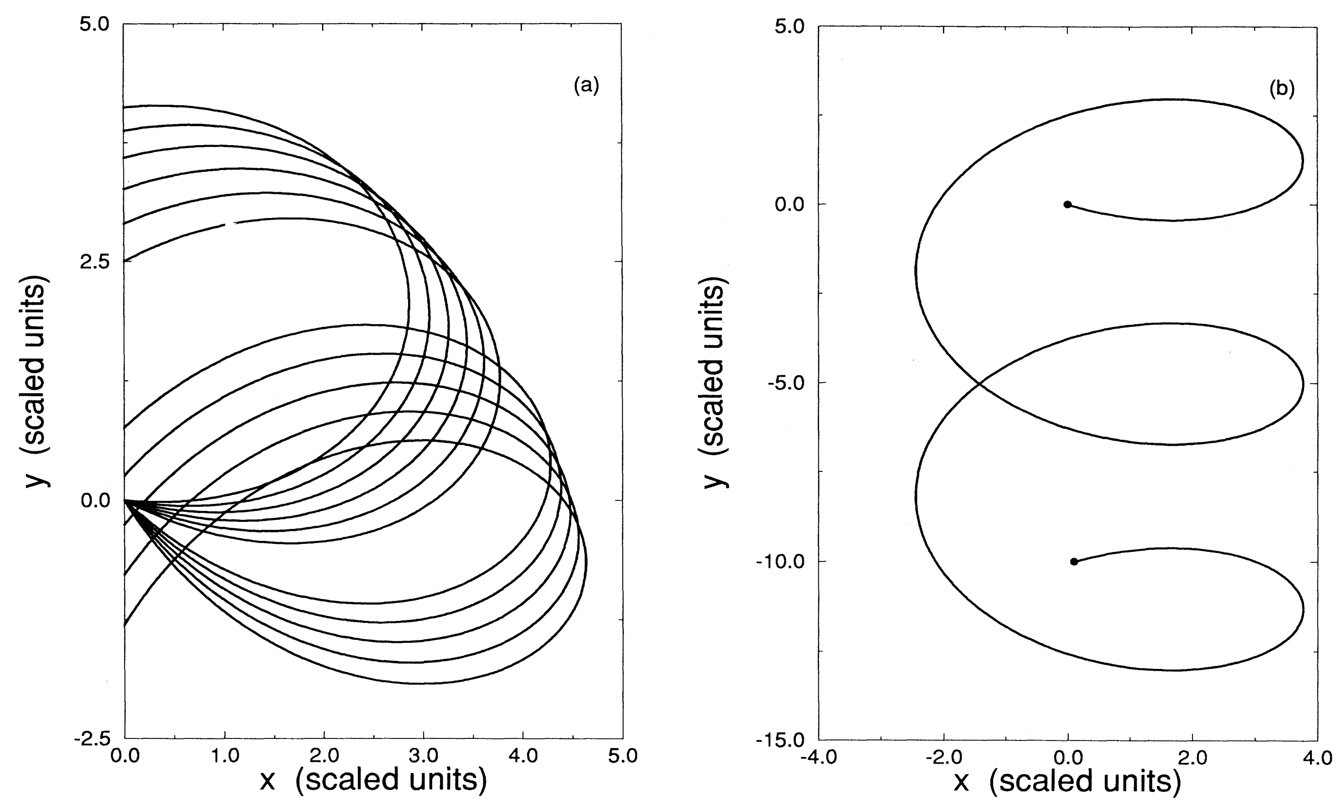

FIG. 1. (a) A family of trajectories in the x-y plane. Each trajectory starts at the origin with the same speed, with initial angle $\theta_0=\pi/2$, $-\pi/2<\varphi_0<\pi/2$, so the initial x component of the momentum is positive. Each trajectory runs until it intersects $x=0$ the first time. The action along this trajectory is given by Eq. (4.17). (b) One trajectory has been continued through one or more cyclotron periods (in this case, two), and again we stop it when it intersects the x axis with $p_x<0$. The action integral along this second path is given by Eq. (4.18).

The function $S_{x,K}$ defined in Eq. (4.19) is precisely the same as the function $S_{x,K}$ defined in Eq. (4.16). Therefore, the stationary-phase points associated with the integral of Eq. (4.12b) are the points where

$$\frac{\partial S_{x,K}}{\partial\theta_0}=\frac{\partial S_{x,K}}{\partial\varphi_0}=0\ . \tag{4.21}$$

Now, from Eq. (4.18), and familiar theorems in classical mechanics, we know that

$$\frac{\partial S_K}{\partial\theta_0}=\frac{\partial S}{\partial y_K}\frac{\partial y_K}{\partial\theta_0}+\frac{\partial S}{\partial z_K}\frac{\partial z_K}{\partial\theta_0}=p_y\frac{\partial y_K}{\partial\theta_0}+p_z\frac{\partial z_K}{\partial\theta_0}$$

$$=p_{y_0}\frac{\partial y_K}{\partial\theta_0}+p_{z_0}\frac{\partial z_K}{\partial\theta_0}\ , \tag{4.22a}$$

and similarly

$$\frac{\partial S_K}{\partial\varphi_0}=p_{y_0}\frac{\partial y_K}{\partial\varphi_0}+p_{z_0}\frac{\partial z_K}{\partial\varphi_0}\ . \tag{4.22b}$$

Evaluating derivatives of $S_{y,K}$ and $S_{z,K}$ in the same way, we find from Eq. (4.19)

$$\frac{\partial S_{x,K}}{\partial\theta_0}=-\left[y_K\frac{\partial p_{y_0}}{\partial\theta_0}+z_K\frac{\partial p_{z_0}}{\partial\theta_0}\right]\ , \tag{4.23a}$$

$$\frac{\partial S_{x,K}}{\partial\varphi_0}=-\left[y_K\frac{\partial p_{y_0}}{\partial\varphi_0}+z_K\frac{\partial p_{z_0}}{\partial\varphi_0}\right]\ . \tag{4.23b}$$

The stationary-phase condition, $\nabla S_x=0$, can be written in the following manner:

$$\begin{vmatrix} \dfrac{\partial p_{y_0}}{\partial\theta_0} & \dfrac{\partial p_{z_0}}{\partial\theta_0} \\ \dfrac{\partial p_{y_0}}{\partial\varphi_0} & \dfrac{\partial p_{z_0}}{\partial\varphi_0}\end{vmatrix}\begin{vmatrix} y_K \\ z_K\end{vmatrix}=\begin{vmatrix}\dfrac{\partial S_{x,K}}{\partial\theta_0} \\ \dfrac{\partial S_{x,K}}{\partial\varphi_0}\end{vmatrix}\ . \tag{4.24}$$

We see that the stationary-phase points of the integral [Eq. (4.12b)] are just where y_K and z_K are zero; that is, at just those values of θ_0 and φ_0 for which the associated orbit returns to the atom after K cycles: stationary-phase points are closed orbits. Furthermore, at those points, $S_{x,K}(p_0,\Omega_0)=S(p_0,\Omega_{\rm sp})$, since $S_{y,K}$ and $S_{z,K}$ vanish at these points.

The determinant involved in the stationary-phase integral is

$$|\det \underline{S}''_{x,K}|=\begin{vmatrix}\dfrac{\partial^2 S_{x,K}}{\partial\theta_0^2} & \dfrac{\partial^2 S_{x,K}}{\partial\theta_0\partial\varphi_0} \\ \dfrac{\partial^2 S_{x,K}}{\partial\varphi_0\partial\theta_0} & \dfrac{\partial^2 S_{x,K}}{\partial\varphi_0^2}\end{vmatrix}\ . \tag{4.25}$$

We evaluate this using

$$\begin{aligned} p_{y_0}&=p_0\sin\theta_0\sin\varphi_0\ ,\\ p_{z_0}&=p_0\cos\theta_0\end{aligned} \tag{4.26}$$

to obtain

$$|\det \underline{S}''_{x,K}|=\begin{vmatrix} p_0\dfrac{\partial z_K}{\partial\theta_0} & 0 \\ 0 & -p_{x_0}\dfrac{\partial y_K}{\partial\varphi_0}\end{vmatrix} \tag{4.27a}$$

$$=\left|p_0p_{x_0}\frac{\partial z_K}{\partial\theta_0}\frac{\partial y_K}{\partial\varphi_0}\right|\ . \tag{4.27b}$$

Let us put Eq. (4.27b) in a more familiar form, relating it to the classical density. The derivative $\partial y_K/\partial\varphi_0$ is evaluated on the final surface, holding x fixed. We may convert it to a partial derivative with t fixed:

$$\left[\frac{\partial y_k}{\partial\varphi_0}\right]_x=\frac{\left[\dfrac{\partial y_k}{\partial\varphi_0}\right]_t\dfrac{\partial x_K}{\partial t}-\dfrac{\partial y_K}{\partial t}\left[\dfrac{\partial x_K}{\partial\varphi_0}\right]_t}{\dfrac{\partial x}{\partial t}}\ , \tag{4.28}$$

so

$$|\det\underline{S}''_{x,K}|=\left|m_ep_0\frac{\partial z_K}{\partial\theta_0}\left[\frac{\partial(x_K,y_K)}{\partial(t,\varphi_0)}\right]\right|\ . \tag{4.29}$$

Let us recall the classical-density Jacobian used in the first paper,

$$J(t)=\frac{\partial(x,y,z)}{\partial(t,\theta_0,\varphi_0)}\ . \tag{4.30a}$$

Since on the closed orbit $\partial z/\partial t=0$, and $\partial z/\partial\varphi_0=0$, this Jacobian is

$$|J(t)|=\left|\frac{\partial z}{\partial\theta_0}\frac{\partial(x,y)}{\partial(t,\varphi_0)}\right|\ , \tag{4.30b}$$

so

$$|\underline{S}''_{x,K}|=|m_ep_0J(t)|\ . \tag{4.31}$$

The other quantity needed for the stationary-phase integral is the signature of the matrix $\underline{S}''_{x,K}$: the number of positive eigenvalues minus the number of negative eigenvalues. The partial derivative $\partial z_K/\partial\theta_0$ is always negative, and p_0 and p_{x_0} are positive, so, referring to Eq. (4.27a), the partial derivative of y_K determines the signature of the matrix:

$$\mathrm{sgn}\underline{S}''_{x,K}=-1-\mathrm{sgn}\frac{\partial y_K}{\partial\varphi_0}\ . \tag{4.32}$$

E. Evaluation of the oscillatory term

We write Eq. (4.12a) as

$$\sigma_q^{\rm osc}=(\mp)\sigma_0\frac{3}{4\pi}\frac{1}{2}\mathrm{Im}\int d\Omega\frac{p_q^2}{p_0^2}e^{(i/\hbar)S_{x,K}(p_0,\Omega)-iK\pi}\ . \tag{4.33}$$

There is a stationary-phase point whenever $S_{x,K}$ has vanishing angular derivatives for any K. Using the stationary-phase approximation,

$$\sigma_q^{\rm osc}=(\mp)\sigma_0\frac{3}{4\pi}\frac{1}{2}{\rm Im}\left\{\frac{p_{q_{\rm ret}}^2}{p_0^2}e^{(i/\hbar)S_{x,K}(p_0,\Omega_{\rm ret})}\times\frac{2\pi\hbar}{|\det\underline{S}''_{x,K}|^{1/2}}e^{i(\pi/4){\rm sgn}\underline{S}''_{x,K}}\right\}, \tag{4.34}$$

and substituting in the various results, we obtain

$$\sigma_q^{\rm osc}=(\mp)\sigma_0 3\sum_{\rm ret}\frac{p_{q_{\rm ret}}^2}{p_0^2}\frac{\hbar}{|m_e p_0 J(t)|^{1/2}}\times\sin\left[\frac{1}{\hbar}S(p_0,\Omega_{\rm ret})-K\pi+\frac{\pi}{4}{\rm sgn}\underline{S}''_{x,K}\right]. \tag{4.35}$$

This is equivalent to Eq. (2.35) of the accompanying paper. Use Eq. (4.30b) of this paper to calculate the Jacobian at $t=0$. Then, referring to the first paper, use Eqs. (2.12), (2.17), and (2.35) [see also (4.2)]. Upon substitution one arrives at the above equation for $\sigma_q^{\rm osc}$, where

$$-\mu_j\frac{\pi}{2}=-K\pi+\frac{\pi}{4}{\rm sgn}\underline{S}''_{x,K}\ . \tag{4.36}$$

Thus we have directly reduced the quantum formulas to the formulas of the closed-orbit theory.

F. Concluding remarks

In the fully quantum framework, the only obvious energy scale is set by the spacing of the cyclotron levels, $\hbar\omega_B$. Accordingly, one might expect that the oscillations in the photodetachment spectrum are spaced by $\hbar\omega_B$. In fact, however, the first set of oscillations have a spacing more than twice $\hbar\omega_B$, the second set are comparable to $\hbar\omega_B$, and the third and higher sets of oscillations are successively shorter, until structure exists on a scale much less than $\hbar\omega_B$. This may be surprising from the quantum viewpoint. However, in the semiclassical theory, we know that the oscillations are related to $\partial S_K/\partial E=T_K\simeq 2\pi K/\omega_B$. The return times vary from somewhat less than to much more than the cyclotron time. In closed-orbit theory, the oscillations have a logical structure that is easy to understand.

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