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Photodetachment cross section of S^- in electric and magnetic fields*

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In this paper, the quantum-mechanical photodetachment cross section of S^- in uniform electric and magnetic fields at arbitrary angles is presented. It compares the quantum-mechanical cross section with the quantum source formalism cross section. The results show that at large angle, the two results have good agreements, however, with the decrease of the angles, they deviate obviously from each other. The reasons for this discrepancy are also discussed.

Keywords: photodetachment cross section, quantum source picture
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Photodetachment can be considered as a collision between an electron and a neutral atom. The aim of the photodetachment study is to analyse the electron correlation effects and other electron–atom interactions. One method to enhance the photodetachment study is to add external electric and magnetic fields. The effect of the external fields is to cause a portion of the out-going electron wavefunction to return to the atomic core, where additional interactions may take place. In recent years, a large amount of attention has been given to calculate the photodetachment cross section of negative ions in the presence of external fields.[1−5] As for the photodetachment of the negative sulfur ion, many researches have studied intensely both theoretically and experimentally. Rau and Wong[6] studied the photodetachment of S^- in an electric field, Blumberg and his co-workers calculated the photodetachment cross section of S^- in magnetic fields.[7,8] Yukich *et al* observed the photodetachment of S^- in parallel electric and magnetic fields and analysed the influence of the time-dependent external field on the photodetachment cross section of S^-.[9] As for the quantum-mechanical cross section of S^- in electric and magnetic fields with arbitrary orientation, none has given the calculation quantum-mechanically.

In this paper, we present the general quantum-mechanical formula for the photodetachment cross section of S^- in the uniform electric and magnetic fields at arbitrary angles. As in the previous study of the photodetachment of S^-,[6] we restrict ourselves to the region around the threshold for this process: $s^- + hv \rightarrow s + e$. We give the cross section as a function of photon energy and the external electric and magnetic fields and compare our quantum-mechanical cross section with the results calculated by using the formula given in Ref.[9].

As in the earlier treatments, we assume the effects of the external fields to be so small in the region close to the atomic core that their influence can be neglected, and the short-range interaction $V_s(r)$ between the photoelectron and the neutral atomic dominates, the initial wavefunction $\Psi_i(\boldsymbol{r})$ is given in Ref.[1]: $\Psi_i = B_0 \dfrac{e^{-ik_B r}}{r}$, in which k_B is related to the binding of the S^-, $E_B = \dfrac{1}{2}k_B^2 = 2.0771\,\text{eV}$. After the active electron absorbs a photon, it is detached from the atomic core and then travels quickly away from the region close to the core, entered the region where the short-range interaction can be neglected and the external fields cannot. In this region, the Schrödinger equation is separable. We assume that the magnetic field $\boldsymbol{H}$ is along the positive-z axis and the electric field $\boldsymbol{F}$ is 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:

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$$\begin{cases} F_1 = F\sin\alpha, \\ F_2 = F\cos\alpha. \end{cases} \tag{1}$$

Then the Hamiltonian for an electron in the combination of electric and magnetic fields is (in atomic units)

$$H = \frac{1}{2}\left[\boldsymbol{P} - \frac{\boldsymbol{A}}{c}\right]^2 + F_1 x + F_2 z, \tag{2}$$

$\boldsymbol{A}$ is the vector potential of the magnetic field ($A_x = A_z = 0, A_y = -Hy$). By inserting the components of $\boldsymbol{A}$ into the above equation, we get

$$\begin{aligned} H = \ & \frac{1}{2}P_x^2 + \frac{1}{2}\omega_{\rm B}^2\left[x + \frac{1}{\omega_{\rm B}}\left(P_y + \frac{F_1}{\omega_{\rm B}}\right)\right]^2 \\ & - \frac{F_1}{\omega_{\rm B}}P_y - \frac{1}{2}\left(\frac{F_1}{\omega_{\rm B}}\right)^2 + \frac{1}{2}P_z^2 + F_2 z. \end{aligned} \tag{3}$$

After solving the Schrödinger equation, we can get the final state wavefunction:[5]

$$\Psi_{\rm f}(\boldsymbol{r}) = \varphi_{\rm n}(x)\mathrm{e}^{\mathrm{i}P_{y0}y}\varphi_z(z), \tag{4}$$

where

$$\varphi_{\rm n}(x) = \left[\left(\frac{\omega_{\rm B}}{\pi}\right)^{\frac{1}{2}}\frac{1}{2^n n!}\right]^{\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}X^2}H_n(X), \tag{5}$$

in which $X = \sqrt{\omega_{\rm B}}\left[x + \frac{1}{\omega_{\rm B}}\left(P_{y0} + \frac{F_1}{\omega_{\rm B}}\right)\right]$, $H_n(X)$ is the Hermite polynomial of order n, and

$$\varphi_z(z) = \left[\frac{4}{F_2}\right]^{1/6}\mathrm{Ai}\left[(2F_2)^{1/3}\left(z - \frac{E_{z0}}{F_2}\right)\right]. \tag{6}$$

The total energy of the final state is

$$E_{\rm f} = \left(n + \frac{1}{2}\right)\omega_{\rm B} - \frac{F_1}{\omega_{\rm B}}P_{y0} - \frac{1}{2}\left(\frac{F_1}{\omega_{\rm B}}\right)^2 + E_{z0}. \tag{7}$$

The photodetachment cross section for any linear polarization is related to the transition dipole matrix element from the initial bound state $\Psi_{\rm i}(\boldsymbol{r})$ to the final state $\Psi_{\rm f}(\boldsymbol{r})$ by

$$\begin{aligned} \sigma_{\rm i\to f}(E) = \ & \frac{2\pi}{c}\int 2E_{\rm p}\delta(E_{\rm f} - E)| < \Psi_{\rm f}(\boldsymbol{r}) \\ & \times |D|\,\Psi_{\rm i}(\boldsymbol{r}) > |^2 \mathrm{d}^3\boldsymbol{r}, \end{aligned} \tag{8}$$

where D is the "dipole-coordinate" operator, and $E_{\rm p}$ is the energy of the photon, which is equal to the sum of the binding energy $E_{\rm B}$ and the final energy E of the electron: $E_{\rm p} = E_{\rm B} + E$.

In the quantum source picture, the motion of a photoelectron that is emitted with an initial kinetic energy E close to zero is governed by the modified Schrödinger equation:

$$\{E - H(\boldsymbol{r}, \boldsymbol{P})\}\,\Psi(\boldsymbol{r}) = C\delta(\boldsymbol{r}), \tag{9}$$

where C is the source strength parameter. The solution of Eq.(9) is given by the energy Green function $G(\boldsymbol{r}, \boldsymbol{o}; E)$ describing an outgoing wave in the external field potential:[10]

$$\Psi(\boldsymbol{r}) = CG(\boldsymbol{r}, \boldsymbol{o}; E). \tag{10}$$

The energy Green function is linked to the familiar time-dependent quantum propagator $K(\boldsymbol{r}, t|\boldsymbol{o}, 0)$ by a Laplace transformation:

$$G(\boldsymbol{r}, \boldsymbol{o}, E) = -\mathrm{i}\int_0^\infty \mathrm{d}t\mathrm{e}^{\mathrm{i}Et}K(\boldsymbol{r}, t|\boldsymbol{o}, 0). \tag{11}$$

By inserting the quantum propagator of electrons in uniform electric and magnetic fields at arbitrary angles,[11] the photodetachment cross section is given by

$$\begin{aligned} \sigma(E) = \ & -\omega_{\rm B}(2\pi)^{-3/2}|C|^2 \times \mathrm{Im}\left[\int_0^\infty \frac{\mathrm{d}t}{\sqrt{\mathrm{i}t}\sin(2\omega_{\rm B}t)}\right. \\ & \left. \times \exp\left\{\mathrm{i}\left(Et - \frac{F_1^2 t^3}{24} + \frac{F_2^2 t}{32\omega_{\rm B}^2}[2\omega_{\rm B}t\cot(2\omega_{\rm B}t) - 1]\right)\right\}\right]. \end{aligned} \tag{12}$$

In the following, taking the energy E to be 0 to 0.5 meV, and the electric and magnetic fields to be 1400 V/m and 1.07 T, respectively, we calculate the cross section for several angles between the fields by using both the quantum mechanical formula and the cross section given by Eq.(12). The spectra are oscillating with the energy (the zero-field cross section σ_0 are omitted.). Figure 1 is the photodetachment cross section of S^- in electric and magnetic fields with the angle of the fields being 85°, Fig.2 is the angle being 45°, while Fig.3 is the angle being 5°.

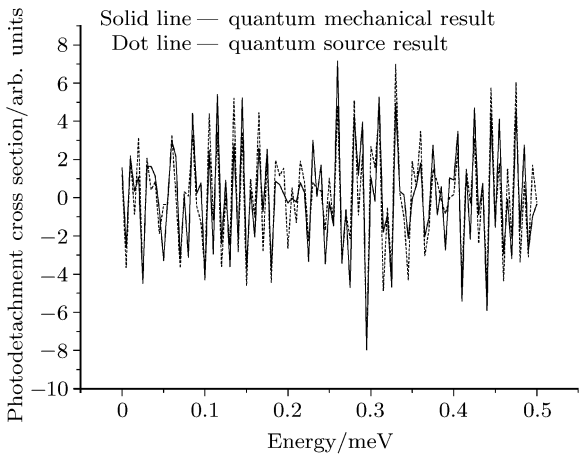


Fig.1. Photodetachment cross section of S^- in the electric and magnetic fields with the angle of the fields being 85°.

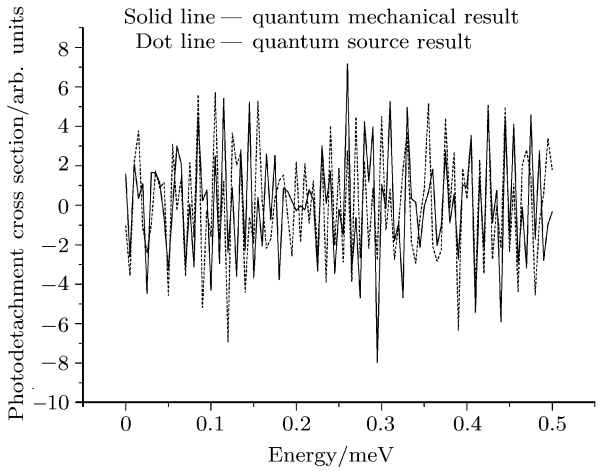


Fig.2. Photodetachment cross section of S^- in the electric and magnetic fields with the angle of the fields being 45°.

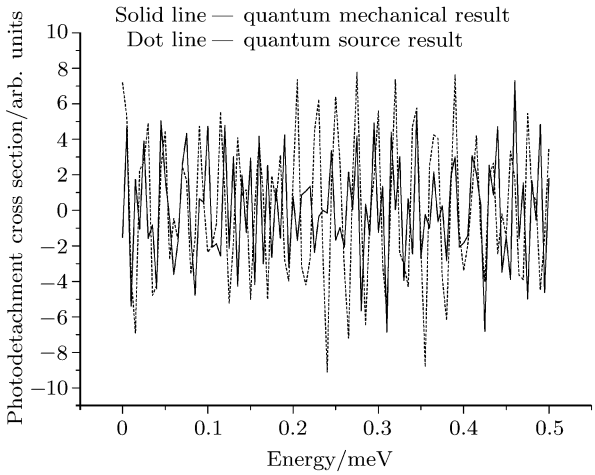


Fig.3. Photodetachment cross section of S^- in the electric and magnetic fields with the angle of the fields being 5°.

From the figures we can see: at large angle, for example, $\alpha = 85°$, the two results agreed well with each other, with the decrease of the angles, the quantum source result deviates obviously from the quantum-mechanical result. As the angle is very small (for example at $\alpha = 5°$, see Fig.3), the two results deviate greatly from each other. The amplitude of the quantum source model cross section is larger than the quantum-mechanical result. The reasons can be analysed as follows. In the analysis of the photodetachment cross section of S^- with the quantum source formalism, the photodetachment can be thought as a collision between the electron and a neutral atom. The effect of the external field is to cause a part of the outgoing electron wavefunction to return to the atomic core, where interference occurs. The interference gives rise to the oscillatory structure in the detachment cross section. The oscillatory structure occurs in the presence of a magnetic field is much more stronger than that produced by an electric field because the magnetic field confines the electron in two dimensions, and consequently a larger portion of the wavefunction returns to the core. The electric field perpendicular to the magnetic field causes the electron to drift away from the core, thus diminishes the interference structure of the photodetachment cross section. But when the angle is very small, the electric field component perpendicular to the magnetic field is very large, which decreases the oscillating structure of the cross section. On the other hand, in the quantum source formalism cross section, we have made some approximations to the Green function, which can also give rise to error.

In summary, we have calculated the cross section of f S^- in uniform electric and magnetic fields at arbitrary angles by using both the quantum-mechanical photodetachment cross section and the quantum source formalism cross section. The results show that at large angles, the two results have good agreements, but with the decrease of the angles, they deviate obviously from each other. Since up to date, no one has given the experimental result, we hope our result will guide future research.

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