ANALYSIS OF THE DIFFERENTIAL CROSS SECTION
FOR EXCITATION OF A HYDROGEN ATOM
BY FAST ELECTRONS IN A UNIFORM ELECTRIC FIELD

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Abstract

The differential cross sections for excitation of a hydrogen atom by fast electrons in an external uniform electric field are calculated using the nonrelativistic Born approximation. It is shown that the cross section obtained can differ substantially from a similar excitation cross section of an almost isolated atom (when the interference of electrons in the course of their reflection from the potential barrier of the external electric field is absent) in the angular distribution of primary electrons in momentum space, oscillation terms, and magnitude.

1. Introduction

The collisions of electrons with atoms and ions in an external uniform quasi-steady electric field can differ significantly from collisions with an isolated atom even when the external electric field is far below the atomic field. This is explained by the interference and the change in the time the electrons stay in the vicinity of the scattering atom while they are reflected from the potential barrier of the external electric field. These effects come into play if the distance between the atomic nucleus and the reflection point of the electrons and the mean time the electrons stay in this region are shorter than the spatial and temporal scales of the problem. This case was considered in [1-3], where, in particular, the differential cross section for ionization of a hydrogen atom by fast electrons in a uniform electric field was calculated using the nonrelativistic Born approximation. When calculating the cross section, the asymptotes of the wave functions of the final electron states were taken in the form of standing waves (along the external electric field) in the region between the atom nucleus and the reflection point of the electrons and in the form of progressive waves in the region where reflection points were absent [1]. Evidently, such wave functions describe the density of the electron current in a weakly ionized gas in an external electric field or in a plasma region with a linear size on the order of the Debye radius where a sufficiently strong electric field exists. Since mathematical expressions for the atom-ionization cross sections were obtained and analyzed numerically in [1-3].

The numerical results show that the cross section for ionization of a hydrogen atom by fast electrons in a uniform electric field can be substantially larger than a similar ionization cross section of an isolated atom, as well as that of an atom in a uniform electric field, but calculated from asymptotes of the wave functions of the final electron states that have the form of standing waves (along the uniform field) at infinity [4] (such functions were used to describe the final states of photoelectrons in [5, 6]) and which are thus inapplicable for describing the density of the electron current with a nonzero longitudinal component.
In this paper, the differential cross section for excitation of a hydrogen atom by fast electrons in a uniform electric field was calculated using the asymptotes of the wave functions which are employed in [1-3] and quantitative study of this cross section was carried out using numerical methods.

2. Formulation of the problem, basic equations

As in [1, 2], we assume that, in a half-space, there is a uniform time-independent electric field \( \varepsilon \) normal to the boundary of the half-space. We assume that the \( z \)-axis of the Cartesian coordinate system \( x, y, \) and \( z \) is antiparallel to the field direction \( (\varepsilon : \varepsilon = (0, 0, -\varepsilon)) \) and a hydrogen-atom nucleus is positioned at the point \((0, 0, 0)\), at a distance \( L \) from the boundary of the region occupied by the field. It is convenient to set the potential of the uniform electric field at this point to be equal to zero.

Let a monoenergetic flow of primary electrons accelerated by the electric field fall from the boundary onto a hydrogen atom, causing its ionization. Keeping in mind that the differential cross section will be calculated in the Born approximation, the wave function for the initial state of a primary electron, constructed from the asymptotes of the Airy functions, can be written in the form

\[
\psi = \frac{A_1}{S^{1/4}} \exp \left\{ \frac{2}{3x_i} \frac{\sqrt{2}}{S^{1/2}} + k_1 z \right\},
\]

where \( A_1 \) is the normalization constant determining the flow density, \( S = +, \ell = m, \) and \( \varepsilon \) are the mass and charge of an electron, \( E_0 = + e \varepsilon L \) is the electron longitudinal energy, and the wave vector \( \chi = (x_i, x) \) determines the electron momentum \( \chi \) at the field boundary. Functions (1) also describe the final states of primary electrons, provided that

\[
E_0 > e \varepsilon L
\]

and the normalization constant \( A \) enters the expression for the number of states referred to the volume element \( d^3x \) of the \( x \)-space [1-4]. If the longitudinal electron energy in the final state is less than \( e \varepsilon L \) \((E_0 < e \varepsilon L)\), then, according to the considerations given in the Introduction, in the Born approximation, the electron motion along the field between the reflection point \( z_r = -E_0/e \varepsilon \) and the atom nucleus must be described everywhere by a finite and real Airy function decreasing exponentially at \( z \rightarrow z_r \). At the same time, in the half-space \( z > 0 \), the longitudinal component of the electron flow density in the uniform electric field obviously must differ from zero and, consequently, the wave-function asymptote in this half-space must take form (1) and correspond to a progressive wave (see [1] for details).

If the inequalities

\[
e \varepsilon L << E_0 << e \varepsilon L
\]

hold, we can neglect the interaction between the electrons and atom nucleus and use the asymptotes of Airy functions. Thus, the wave function \( \psi_b \) for the classically permitted region of motion can be written in the following form [1]:

\[
\psi_b = \frac{A_b}{S^{1/4}} \exp(k_1 z)
\begin{cases} 
\sin \left( \frac{2}{3} \frac{\sqrt{2}}{S^{1/2}} + \alpha_1 \right) & \text{for } z, < z < 0 \\
\exp \left( \frac{2}{3} \frac{\sqrt{2}}{S^{1/2}} + \alpha_2 \right) & \text{for } z > 0
\end{cases}
\]

where the phases \( \alpha_1 \) and \( \alpha_2 \) should be regarded as fitting parameters that, presumably, are close to \( \pi/4 \); \( A_b \) is the normalization constant related to the number of electron states \( d \theta \) referred to
the element volume $d^4k$ of the $k$-space by the equation $d^4k = (|k| / 8 \pi^3 |d^3k|) d^4k$; and $k = (k_1, (2m_eE_z) / \hbar^2)$ is the local wave vector determining the electron momentum in the vicinity of the nucleus. Assuming that a low (compared to the atomic field) external uniform electric field switches on adiabatically slowly, the initial state of the atom electron is described by the wave function \( \Psi_0 \) of an isolated atom:

\[
\Psi_0 = \left( \frac{\pi a^3}{\hbar} \right)^{-1/2} \exp(-r_2/a),
\]

where \( r_2 \) is the radius vector of the atom electron and \( \alpha = \hbar^2 / (m_e e^2) \).

In this paper we examine transition to the atom electron excitation states which are described by the wave functions of zero approximation:

\[
\Psi_0 = (2) \exp(\i k_1 x_1),
\]

where \( k = \pm 1 \); \( \Psi_{2s} = \frac{1}{4\sqrt{2}} \left( 2 \frac{r_2}{a} \right) \exp(-2 \frac{r_2}{a}) \); \( \Psi_{2p} = \frac{1}{4\sqrt{2}} \left( 2 \frac{r_2}{a} \right) \exp(-2 \frac{r_2}{a}) \).

The correspondant energies (to the first approximation) of the electrons in these states are

\[
-\frac{e^4 m_e}{8\hbar^2} - 3e\alpha \hbar \Omega.\]

Using (1), (4), (5) and (6) for the wave functions of the initial and final electron states, we obtain the following expression for the differential cross section \( d\sigma_x \) for excitation of a hydrogen atom by fast electrons in a uniform electric field (in atomic units):

\[
d\sigma_x = 16(k_0, k_1) |T_x|^2 d\Omega,
\]

where \( k_0 \) and \( k_1 \) are the wave vectors of the initial and final states of the primary electron, respectively. Here, we assume that \( k_0 \) lies in the $xz$ plane, \( k_1 = k_0 - 3/4 + 6k \); \( d\Omega = \sin\theta d\theta d\varphi \), the angles \( \theta, \varphi \), were defined as follows: \( \theta \) between \( k_0 \) and the vectors \( k \); \( \varphi \) between the vector \( k_0 = \hat{z} \) (here, \( \hat{z} = k_0 \hat{z} \) and \( \hat{z} \) is the unit vector in the direction along the $y$-axis) and projection of the vector \( \hat{z} \) onto the plane formed by the vectors \( k_0 \) and \( j \).

The expression for \( T_x \) takes a different form depending on the relation between \( k_0 \) and \( j, l, t \). If the inequalities \( \epsilon_{13, t} \ll k_0 \ll 2 \) \( \ll eL \).

\[
T_x = \frac{2}{q^2} \left( \frac{1}{9 + 4q^2} \right)^2 \left[ \frac{16 \cdot 2q^2 + 3iq_{12} \cdot 2x}{9 + 4q^2} \left( e^{-m} - \frac{i}{2} e^{-m} \right) + 9 \left( \frac{9 + 4q^2}{9 + 4q^2} \right)^2 \left( e^{-m} - \frac{i}{2} e^{-m} \right) \right] -
\]

\[
\frac{i e^m}{q} \left( \frac{1}{9 + 4q^2} \right)^2 \left[ \frac{16 \cdot 2q^2 - 3iq_{12} \cdot 2x}{9 + 4q^2} \left( e^{-m} - \frac{i}{2} e^{-m} \right) + 9 \left( \frac{9 + 4q^2}{9 + 4q^2} \right)^2 \left( e^{-m} - \frac{i}{2} e^{-m} \right) \right] +
\]

\[
\frac{1}{3} \left( \frac{4q_0}{9 + 4q^2} \right)^2 \left( h_1 + h_2 \right) + \frac{6q_0}{9 + 4q^2} \left( h_1 - h_2 \right); \]

\[
\bar{q}_1 = \bar{x} = \bar{k}_1 = \bar{k}_2; \bar{x}_1 = \bar{x}_2 = \bar{k}_1 \pm \bar{k}_2; \]

\[
R_1 = 1 + \frac{iq_{12}}{\sqrt{9 + 4q^2} \left( 3 + 4q^2 \right)} \left( 3 + 4q^2 \right); \]

\[
P = 1 - \frac{q_{12}}{\sqrt{9 + 4q^2} \left( 3 + 4q^2 \right)} \left( 3 + 4q^2 \right); \]

\[
k_1 = k \cos \theta \sin \theta, \cos \varphi + \sin \theta \cos \theta; \]

\[
k_2 = k \sin \theta \sin \varphi; \]
\[ k_{xx} = \pm k (\cos \theta \sin \theta \cos \varphi + \sin \theta \cos \varphi) \]  \( \bar{k}_e = k (\sin \theta_0 \cos \theta_0) \)

When \( k_e^2 / 2 > \varepsilon L \), we have

\[ T_1 = \frac{64}{q^2 \left( 9 + 4q^2 \right)^{\frac{3}{2}}} \left( 2q^2 - 3izq_{zz} \right) \]

3. Numerical analysis of cross sections

The cross sections \( d\sigma \) are analyzed numerically by representing the functions \( F = d\sigma / d\omega \) in the form of surfaces constructed on the planes (the white strips on the coordinate planes show the regions in which the obtained formulas are inapplicable) with coordinates corresponding to the parameters entering the formula for \( d\sigma \).

For the numerical analysis, we set \( \varepsilon = 0.01, L = 10^4, k_e = 51 \) and the phases \( \alpha_1, \alpha_2 \), to be equal to 0.78\( \pi / 4 \) (the angles are given in radians).

We begin the analysis of the function \( F \) with the case \( \theta_0 = 1.5 \) when the momentum of the electrons incident on the atom are directed almost perpendicular to the vector \( \varepsilon \) (according to the applicability conditions for the expressions obtained for \( d\sigma \)). Figure 1 shows this surface and its fragment of the function \( F(\theta, \varphi) \) in the intervals (0.1, 0.104) and (1.3, 1.308) of the angles \( \theta \) and \( \varphi \).

It follows from this figure that the fragments of the function \( F(\theta, \varphi) \) have an oscillatory structure and vary from 0.014 to 0.035 with a period of 0.001 (along \( \varphi \)).

Fig. 1 Functions \( F(\theta, \varphi) \) and their fragments calculated for \( k_e = 51 \) and \( \theta_0 = 1.5 \): (a) \( F_{\text{max}}(\theta, \varphi) = 2.07 \) for \( \kappa = -1 \) and \( F_{\text{max}}(\theta, \varphi) = 3.36 \) for \( \kappa = 1 \); (b) \( F(\theta, \varphi) \) varying from 0.014 to 0.035 in the intervals (0.1, 0.104) and (1.3, 1.308) of the angles \( \theta \) and \( \varphi \), respectively (\( \kappa = \pm 1 \)).

Fig. 2. Functions \( F(\theta, \varphi) \) and their fragments calculated for \( k_e = 51 \) and \( \theta_0 = 0 \): (a) \( F_{\text{max}}(\theta, \varphi) = 17590.72 \) for \( \kappa = -1 \) and \( F_{\text{max}}(\theta, \varphi) = 24242.95 \) for \( \kappa = 1 \); (b) \( F(\theta, \varphi) \) varying from 0.00002 to 0.00014 in the intervals (1.552, 1.56) and (−8, 8) of the angles \( \theta \) and \( \varphi \), respectively (\( \kappa = \pm 1 \)).

In this case, the other characteristic value of the angle \( \theta_0 \) are 0 (when the momenta of the primary electrons in their initial states are antiparallel to \( \varepsilon \)). Figure 2 shows the surface \( F(\theta, \varphi) \) and its fragment corresponding to this value of the angle \( \theta_0 \).
It follows from this figure that the fragments of the function $F(\theta, \varphi)$ have an oscillatory structure and vary from 0.00002 to 0.00014 with a period of 0.001 (along $\theta$). This is explained by the form of the expression for $T$, which contains oscillatory terms dependent on $k_e$ when $\varepsilon \lambda \sim E_0$ and the electrons reflect from the potential barrier of the uniform electric field.

In order to compare this cross sections with a similar cross sections for excitation of an atom Fig. 3 illustrates these surfaces of $F_0(\theta, \varphi)$ for $\theta_0 = 1.5$ and for $\theta_0 = 0$ when the interference of electrons is absent (but $\varepsilon = 0$).

![Diagram showing oscillatory structure](image)

Fig. 3. Functions $F(\theta, \varphi)$ and their fragments calculated for $k_e = 51$, $\theta_0 = 1.5$ and $\theta_0 = 0$: (a) $\theta_0 = 1.5$: $F_{\text{max}}(\theta, \varphi) = 5990$ 14 for $\varepsilon = \pm 1$; (b) $\theta_0 = 0$: $F_{\text{max}}(\theta, \varphi) = 20518.56$ ($\varepsilon = \pm 1$).

The functions $F_0(\theta, \varphi)$ have not an oscillatory structures. This is explained by the form of the expression for $T$, which contains no oscillatory terms dependent on $k_e$ when $\varepsilon \lambda < E_0$ and the electrons do not reflect from the potential barrier of the uniform electric field.

It easily seen from the shape of the surfaces shown in these figures that the functions $F_0(\theta, \varphi)$ and especially $F(\theta, \varphi)$ depend strongly on the angle $\theta_0$. This anisotropy that appears in the cross section is due to the uniform electric field.

4. Conclusion

It is expected from the above considerations that the differential cross section for excitation of a hydrogen atom by fast electrons in an external uniform electric field can differ significantly from a similar excitation cross section of an almost isolated atom in both the angular dependence and magnitude. The most pronounced increase in the cross section is expected if the atom is excited by electrons with momentums directed almost perpendicularly to the uniform electric field. The cross section under consideration contains oscillation terms whose periods depend on the longitudinal energy of primary electrons. The anisotropy that appears in the cross section is due to the uniform electric field.

The physical explanation for these effects is the redistribution (in comparison with the case $\varepsilon = 0$) of the mean electron density when the electrons are reflected from the potential barrier of the external electric field. In ionized gases, these effects should appear when the distance between the scattering-atom nucleus and the point of the electron reflection from the potential barrier of the uniform electric field is shorter than the mean distance between ions or gas atoms: $E < \varepsilon n^{1/3}$ (here, $n$ is the density) and the mean time $\tau \sim (m_eE)^{1/2}/e\varepsilon$ needed for the electrons to pass over this distance is much shorter than the characteristic time of the process under study. Assuming $E = 1 \text{ eV}$ and $n = 10^{12} \text{ cm}^{-3}$, we obtain $\varepsilon \approx 10^4 \text{ V/cm}$ and $\tau < 10^{-11}$. Hence, it is expected that, if a gas with a density of $10^{12} \text{ cm}^{-3}$ is in an alternating electric field...
field with frequency \( \omega < 10^{12} \text{s}^{-1} \) and amplitude on the order of \( 10^2 \text{kV/cm} \), the above effects should come into play.

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References