Photoionization of hydrogen molecular ion by ultrashort photo-pulse in a wide range of field magnitudes

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Abstract. The probabilities of photoionization of hydrogen molecular ion by ultrashort laser field were evaluated on base of earlier developed trajectory method. The results are obtained in a wide range of field magnitudes up to superatomic fields approaching relativistic intensities. In a weak field gained results are in good agreement with the data obtained by other methods. In a strong field the photoionization probability behaviour resembles some features of the so called stabilization effect in atoms.

1. Introduction
The process of photoionization of atoms and molecules is of great importance in various plasma media, for example, in astrophysical plasma, where hydrogen is of especial interest ([1]; also see bibliography in [2]). It has been studied for a long time, however the interest to this process resumed in connection with development of ultrafast strong field radiation sources. There are several theoretical approaches to address this problem [3]. In this respect the trajectory based method for calculating transition probabilities in a quantum system developed in our works [4–9] has many advantages. It can be treated as the variant of semiclassical approximation in Weyl representation. The method is nonperturbative and takes into account all orders of multiphoton and recollision processes. It takes into account electron's correlations for multielectron systems. The photoionization probabilities can be calculated in a wide range of field frequencies and intensities. It makes possible to evaluate photoionization probability directly for entire ionization continuum without integration over probabilities for each state in continuum. Computation of each continuum state (especially for multielectron system) may be rather complicated problem. At the same time total ionization probability is often required in practice. The possession of totality of these capabilities is unique compared to the other methods.

2. Method
The transition probability \( w \) is calculated as follows (atomic units are used throughout the paper if not stated otherwise)

\[
w(t',t) = \frac{1}{\nu} \int W_f(\zeta) \left| \exp(i S(\zeta)) - K(t',t) \right|^2 W_i(\zeta_0) d\zeta_0 ,
\]

\[
K(t',t) = \frac{1}{\nu'} \int \exp(i S(\zeta)) W_i(\zeta_0) d\zeta_0 ,
\]
where \( v = (2\pi)^n \) is the quantum unit volume of the phase space, \( 2n \) is the phase space dimension, \( t' \) and \( t \) are the initial and final moments in time, respectively, \( W_i \) and \( W_f \) are the Weyl’s symbols of initial and final states, respectively, 
\[
S(\zeta) = \int_{t'}^t V dt 
\]
is the integral of the interaction \( V \) (the phase function) taken along stationary phase trajectory \( \zeta = (q, p) \) from the initial point \( \zeta_0 = (q_0, p_0) \) to the final one \( \zeta_f = (q_f, p_f) \). These trajectories are solutions of the Hamilton’s equations with initial phase space coordinate \( \zeta_0 \). The parameter \( K(t', t) \) (2) excludes contribution of the system evolution without interaction.

In this paper we apply this method in calculating the probabilities of hydrogen molecular ion photoionization under the exposure of ultrashort laser radiation. The results are represented for equilibrium internuclear distance (\( R = 2 \)).

The Weyl symbol \( W_i \) of the ground electronic state in hydrogen molecular ion was evaluated using the wave functions taken from the works [10, 11]. We consider transitions into all inelastic channels and into entire continuum. Final states can be represented by means of the projectors on corresponding groups of states. Note that the projector on the whole set of all eigenstates of Hamiltonian \( \hat{H}_0 \) for the system without interaction is equal to the identity operator due to the completeness of the set. The Weyl’s symbol of identity operator is equal to one
\[
W_f(\zeta) = 1.
\]
The usage of this symbol in (1) yields the total probability of all inelastic transitions since the transition into initial state is excluded by means of parameter (2). The projector into entire continuum can be represented by subtracting from the identity operator the projector to all states of the discrete spectrum. So it is reasonable to introduce the following model of the final distribution excluding the energy gap containing discrete levels which in boolean notation reads as
\[
W_f(\zeta) = H_0(\zeta) < \epsilon_0 \lor \epsilon_1 < H_0(\zeta),
\]
where \( \epsilon_0 = -0.67, \epsilon_1 = 0 \) are the energies of the first excited state of hydrogen molecular ion and its ion respectively. Such model distribution was tested in our works [4–6] and had given reliable results.

Interaction of a system (of electrons) with an electromagnetic field in velocity gauge can be written up to the second relativistic order as
\[
V(r, p, t) = \frac{e}{mc} p \cdot A(r, t) - \frac{e^2}{2mc^2} A^2(r, t),
\]
where \( A \) is a vector potential and \( r \) and \( p \) are coordinate and kinetic momentum of electron. We consider a plane-wave photo-pulse with linear polarization and a Gaussian modulation.

3. Results
The result in a weak field is usually represented in a form of cross section. Gained hydrogen molecular ion photoionization cross section averaged over molecular orientations is shown in figure 1.

The calculations are presented for the photon-pulse duration of \( \tau = 50 \) (\( \sim 1.2 \) fs). There are several works with calculations of ionization cross section for a stationary radiation with agreement of results. For example, in figure 1 our results are compared with the data of [12, 13]. Our calculations are in good agreement with the data obtained by other methods especially taking into account the simplicity of our method.
Figure 2 shows photoionization probability dependence on field magnitude. The magnitude of the field is represented by the dimensionless Faisal parameter $\chi = \frac{eA}{p_0c}$ (the ratio of the addition to electron's kinetic momentum in a field $\frac{eA}{c}$ to the atomic scale of electron momentum $p_0 = \frac{\hbar}{a_0}$).

**Figure 1.** $H_2^+$ photoionization cross section $\sigma$(Mb) dependence on photon energy $E$ (eV).
Line 1 – our result, line 2 – [12], line 3 – [13].

**Figure 2.** $H_2^+$ transition probabilities $w$ dependence on Faisal parameter $\chi$: into all inelastic channels (line 1) and into entire continuum (line 2).
If \( \omega \tau >> 1 \) then \( \chi \sim 1/\gamma \), where \( \gamma \) is the Keldysh adiabatic parameter. The range of Faisal parameters \( \chi << 1 \) corresponds to a weak field, \( \chi \sim 1 \) corresponds to an intermediate field, \( 1 < \chi < c \) corresponds to a strong superatomic field, but with lower than relativistic intensities, and \( c < \chi \) to a field with relativistic intensity (\( c = 137 \)).

The calculations are presented for the frequency of the radiation field of \( \omega = 1.1 \) \((\sim 30\text{ eV})\) at ionization threshold, the photon-pulse duration of \( \tau = 50 \) \((\sim 1.2\text{ fs})\) and the wave propagating along molecular axis.

In figure 2 we see how the linear dependence of the probability on the intensity \( \chi^2 \) in a weak field turns into a nonlinear one with a Faisal parameter greater than 0.1. In the field magnitude region \( 0.3 < \chi < 10 \) the photoionization probability behaviour resembles some features of the so called stabilization effect in atoms [14].

4. Conclusions
The probabilities of photoionization of hydrogen molecular ion by ultrashort laser field are obtained in a wide range of field frequencies and magnitudes up to superatomic fields approaching relativistic intensities. It has been found that in a weak field gained results are in good agreement with the data obtained by other methods and in a strong field its behaviour resembles some features of the so called stabilization effect in atoms.

In addition to the studies carried out, it is planned to investigate the dynamics of photoionization.

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