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The prospects of evaluation the probabilities of multiple photoionization of atoms in a wide range of field strengths on base of one method

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ABSTRACT

Theoretical studies of the processes in multielectron atoms under the exposure of strong electromagnetic fields is intensively developed subject in laser physics. Many interesting features of these processes are difficult to be reproduced by means of the existing theoretical methods. It concerns, for example, the effects of electron–electron correlations in multiple photoionization. In light of the progress in this area for weak and strong fields it may be of interest to develop a method equally efficient for a wide range of field strengths. In this paper the capability of a new trajectory-based method, which works in a wide range of field strengths and reproduces effects attributed to electron–electron correlations, is demonstrated for single- and double-photoionization in helium atom.

1. Introduction

The studies of photoionization as a fundamental process is especially relevant in connection with development of ultrafast strong field radiation sources [1,2]. In spite of the progress in theory, many interesting features of these processes are difficult to be reproduced by means of the existing methods, especially in case of multielectron systems.

Helium atom is very convenient object for testing theoretical methods for the interaction of a strong laser field with multielectron atomic systems. Photo-ionization of helium atom was studied by many theoretical methods, including direct numerical solution of time dependent Schrödinger equation [3]. Obviously the last one approach cannot be applied to atoms with more electrons and the need for new approximate schemes with wider capabilities remains. It is especially essential for photo-ionization by strong laser field.

Trajectory methods are a valuable tool in quantum physics. They are widely used when the direct solution of Schroedinger equation is impossible. There are a large number of these methods with different degrees of generality, validity and efficiency [4–15]. In our works [16–18] we developed the trajectory method for evaluation transition probability in quantum system. The variant of this method using Weyl symbols of initial and final states, developed in subsequent work [19], has several advantages.

In this paper we demonstrate the capability of this method in calculating probabilities of single- and double-photoionization of helium atom in a wide range of field strengths. Note that the interpretation of double-photoionization process mechanisms requires an account of electron–electron correlation and gained results shows possibilities of method in this respect.

2. Evaluation method

We rely upon the trajectory-based method for evaluation the transition probability developed in [19]. Atomic units are used throughout the paper. The transition probability is calculated as

$$w_{i,f}(t',t) = \frac{1}{\nu}\int W_f(q_l,p_l)\left|\exp(iS_I) - K\right|^2 W_i(q_0,p_0)dq_0dp_0, \tag{1}$$

$$K = \frac{1}{\nu}\int \exp(iS_I)W_i(q_0,p_0)dq_0dp_0, \tag{2}$$

where $\nu = (2\pi)^n$, n is coordinate space dimension, t', t are initial and final time moments, W_i, W_f are Weyl symbols of initial and final states, $S_I = -\int_{t'}^{t} V dt$ is the integral of the interaction taken

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along stationary phase trajectories (q, p), from the initial points (q_0, p_0) to the final ones (q_l, p_l). These trajectories are solutions of Hamilton equations with initial points (q_0, p_0).

3. Formulation of the problem

In this section we consider some details of application of the scheme based on formulas (1), (2) to the calculation of helium photo-ionization probability.

Interaction of electromagnetic field with an atom in velocity gauge is

$$V(q,p,t) = \frac{1}{c}\sum_j \left(\boldsymbol{p}_j \cdot \boldsymbol{A}(\boldsymbol{r}_j,t) + \frac{1}{2c}\left|\boldsymbol{A}(\boldsymbol{r}_j,t)\right|^2 \right),$$

where $\boldsymbol{A}$ is the vector magnetic potential, $\boldsymbol{r}_j$ and $\boldsymbol{p}_j$ are coordinate and generalized momentum of j-th electron.

A plane wave pulsed field of the shape f with linear polarization propagating along the wave vector $\boldsymbol{k}$ was considered

$$\boldsymbol{A}(\boldsymbol{r},t) = \boldsymbol{e} \cdot A f\big(\varphi(\boldsymbol{r},t)\big), \qquad \varphi(\boldsymbol{r},t) = \boldsymbol{k}\cdot\boldsymbol{r} - \omega\cdot t, \qquad k = \frac{\omega}{c},$$

where $\boldsymbol{A}$ is its amplitude, ω is carrier frequency, $\boldsymbol{e}$ is a unit vector of polarization direction. Electric and magnetic fields can be written as

$$\boldsymbol{E} = k\cdot\boldsymbol{e}\cdot\frac{\partial f}{\partial\varphi}, \qquad \boldsymbol{B} = \boldsymbol{k}\times\boldsymbol{e}\cdot\frac{\partial f}{\partial\varphi}.$$

In our work a pulse with a Gaussian carrier modulation was used

$$f(\varphi) = \exp\left(-\left(\frac{\varphi}{\omega\tau}\right)^2\right)\cos(\varphi),$$

where τ is pulse duration parameter.

The Coulomb potential in atomic Hamilton function was approximated by widely used soft-core potential $\frac{1}{\sqrt{r^2+\delta^2}}$ with parameter δ [20].

We neglected spin–orbital and spin–field interactions and made integration over spin variables in assumption that the detector is insensitive to spin polarization and hence the final spin state is unit spin matrix. More details are in [18].

Initial (ground) state helium orbital wave function was taken as

$$\psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{Z^3}{\pi}\exp\big(-Z(r_1+r_2)\big)$$

with effective nuclear charge $Z = 1.7$ [21]. It is the product of single-electron hydrogen-like functions and its Wigner function (Weyl symbol of the density operator) can be written as the product of the Wigner functions for hydrogen-like states

$$W_i = W\left(Z\boldsymbol{r}_1, \frac{\boldsymbol{p}_1}{Z}\right)W\left(Z\boldsymbol{r}_2, \frac{\boldsymbol{p}_2}{Z}\right),$$

which were calculated using a representation developed in [22].

Note that the choice of initial and final states is a stand alone problem independent of the method. Corresponding Weyl symbols are to be produced separately. Let us consider the integrated ionization probability. So we need the calculation of the Weyl symbol for the group of final states, in particular for the entire ionization continuum. This is rather difficult even for the hydrogen atom. In this paper we consider models of the final distributions.

First note that the whole set of all eigenstates of atomic Hamiltonian $\hat{H}_0$ according to completeness corresponds to identity projector operator with Weyl symbol equal to one

$$W_f(q,p) = 1.$$

The usage of this symbol strictly gives total probability of transitions in all inelastic channels (eigenstates of atomic Hamiltonian $\hat{H}_0$ excluding the initial state) [19].

Our models of the final distribution are based on an atomic Hamilton function. Let us write the helium atomic Hamilton function as

$$H_0(q,p) = H_s(\boldsymbol{r}_1,\boldsymbol{p}_1) + H_s(\boldsymbol{r}_2,\boldsymbol{p}_2) + \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|},$$

$$H_s(\boldsymbol{r}_j,\boldsymbol{p}_j) = \frac{1}{2}p_j^2 - \frac{2}{r_j}.$$

Let us denote $\varepsilon_0 = -2.9$ – helium atom ground state energy and $\varepsilon_1 = -2$, $\varepsilon_2 = 0$ – the ground state energies of single- and double-ionized atom.

Total ionization probability was evaluated with model distribution

$$W_f(q,p) = \begin{vmatrix} 1 & \text{if } H_0(q,p) < \varepsilon_0 \text{ or } \varepsilon_1 < H_0(q,p), \\ 0 & \text{otherwise.} \end{vmatrix} \tag{3}$$

Thus the energy gap containing discrete levels is excluded.

With the introduced function with Boolean value

$$R(q,p) = H_s(\boldsymbol{r}_1,\boldsymbol{p}_1) < \varepsilon_0 \text{ and } H_s(\boldsymbol{r}_2,\boldsymbol{p}_2) < \varepsilon_0$$

single ionization probability was evaluated with model distribution

$$W_f(q,p) = \begin{vmatrix} 1 & \text{if (not } R(q,p) \text{ and } H_0(q,p) < \varepsilon_0) \\ & \quad \text{or } \varepsilon_1 < H_0(q,p) < \varepsilon_2, \\ 0 & \text{otherwise} \end{vmatrix} \tag{4}$$

and double ionization probability was evaluated with model distribution

$$W_f(q,p) = \begin{vmatrix} 1 & \text{if } (R(q,p) \text{ and } H_0(q,p) < \varepsilon_0) \\ & \quad \text{or } \varepsilon_2 < H_0(q,p), \\ 0 & \text{otherwise.} \end{vmatrix} \tag{5}$$

As required for exact Weyl symbols the model distributions (4) and (5) are mutually orthogonal and their sum gives the distribution (3). The advantage of these models is that they have straightforward generalization on atoms with more electrons.

Model distribution (3) was tested by evaluation of total photoionization probabilities in hydrogen and helium atoms in the work [19] and had given reliable results.

Further we consider probabilities in a time domain with $t' = -2\tau$, $t = 2\tau$.

Integrations over initial points in formulas (1), (2) were performed by means of Monte Carlo method.

4. Application examples

First we consider weak field. We calculated photoionization probability dependence on the field carrier frequency ω for the field parameters $A = 10^{-3}$, $\tau = 30$. In weak fields the results are usually represented in form of cross sections which can be evaluated as

$$\sigma = \frac{w}{\tau J},$$

where $J = \frac{P}{\omega}$, $P = \frac{c}{4\pi}E^2$ is Poynting energy flux density.

Results for total photoionization are represented in Fig. 1 and for double photoionization in Fig. 2. A soft-core potential parameter of $\delta = 0.2$ was used. There are several works with single- and double-photoionization of helium [23–30]. The spread of different cross sections is within 10%. Precision experimental data of [23,24] and calculations on base of the hyperspherical R matrix with semiclassical outgoing waves (HRM-SOW) method [26]