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# Evaluation of Total Cross Section of Photo-Ionization of Helium in Weak Field on Base of Trajectory Method

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***Abstract*—**Total cross section of helium atom photo-ionization by weak short pulse is calculated using the variant of trajectory method, developed in our earlier work. The method enables simple estimation of total ionization probability (or cross section) without integration of differential one.

***Keywords*—**Transition probability, cross section, density matrix, atom, photo-ionization.



## I. Introduction

THERE are several approaches for evaluation the transition probability in quantum system based on the trajectory methods. It may be used pure classical or semiclassical theories. The last ones are often treated on base of path integrals. In some cases, schemes using IVR (initial value representation), such as the Herman–Kluk method or other approaches involving wave packets can improve the efficiency of calculations. Related topics are considered in our works [1]-[4]. In particular rather efficient scheme was developed in [3] for evaluation the transition probability in quantum system in case of final state with diagonal density matrix. Such density matrix can be reasonable approximation for the large group of states, for example considered in ionization processes. This method has been successfully tested on hydrogen photo-ionization in case of weak field [3] and for helium photo-ionization by a short intense photo-pulse [4]. Photo-ionization of helium atom was studied by majority of theoretical methods, including direct precise numerical solution of time dependent Schrödinger equation. Obviously the last one approach cannot be applied to atoms with more electrons and the need of approximate schemes with wider capabilities still remains. Our approach claims to be such one. Results for helium photo-ionization illustrate the capabilities of the method to account electron-electron correlations, which is difficult for the majority of theoretical approaches. In present work we apply method for the process of helium photo-ionization by a short weak photo-pulse. Atomic units are used throughout the paper.

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## II. Evaluation Method

Transition probability on time interval $t - t'$ is represented in form

$$w = \int \rho(q_{l+1}) \left|\exp(i\,SI) - K\right|^2 \rho_i(q_0)\, dq_0 \qquad (1)$$

$$K = \int \exp(i\,SI)\, \rho_i(q_0)\, dq_0 \qquad (2)$$

where $\rho_i$, $\rho$ – are diagonal parts of orbital density matrices of initial and final states (probability distributions). $SI = S - S_0$ – is an integral sum for interaction integral

$$SI = -\int_{t'}^{t} V dt$$

Interaction integral is taken on a phase trajectory $(q, p)$ with initial point

$$q_0\,,\ p_0 = \frac{\partial \chi_i}{\partial q_0}$$

where $\chi_i$ – is initial state phase, $q_{l+1}$ is a coordinate of a final point. This trajectory is an extreme value of some functional $\tilde{S}$. It is assumed that complex exponential of this functional includes some generic oscillating part of an integrand in path integral representation of transition probability. Two natural choices of the functional $\tilde{S}$ are $\tilde{S} = S_0$ or $\tilde{S} = S$. where $S$, $S_0$ – are Hamiltonian actions with and without interaction correspondingly

$$S = \int (pdq - Hdt)$$

Our choice of $\tilde{S}$ is close to the second variant and is described in next section.

Advantage of this method is that it belongs to IVR schemes having rather efficient realization. Besides, it does not include the pre-exponent factor with determinant, specific for many

semi-classical schemes. Calculation of this factor is a complicated task in most cases. This method enables simple estimation of total ionization probability without integration of differential probability. Calculation of the last one is complicated by the lack of information about the atomic states in ionization continuum.

## III. Details of the Problem Statement and Results

In this section we apply the scheme based on formulas (1), (2) to calculation of helium photo-ionization cross section in weak laser field.

An electric dipole approximation is used to describe atom interaction with photo-pulse

$$V = -\vec{E}(t)\cdot\vec{D}$$

where $\vec{E}(t)$ – is electric field strength, $\vec{D}$ – is an operator of electric dipole momentum. This leads to restrictions on the light field intensity and carrier frequency, which were satisfied in our work. Photo-pulse with linear polarization is considered

$$\vec{E}(t) = \vec{e}\,F\,\exp\left(-\left(\frac{t}{\tau}\right)^2\right)\sin(\omega t)$$

$F$ – is its amplitude, $\tau$ – is pulse duration parameter, $\omega$ – is carrier frequency, $\vec{e}$ – is a unit vector of polarization direction and Gaussian carrier modulation is chosen.

The cross-section is defined as

$$\sigma = \frac{v}{J}$$

where $v = \frac{w}{\tau}$ is a transition probability per unit time (a transition velocity), $J$ – is photons flux density, which can be estimated by Poynting's energy flux density $P = \frac{c}{4\pi}F^2$ as

$$J = \frac{P}{\hbar\omega}$$

Let's describe diagonal parts of density matrices for initial and final states.

Initial (ground) helium state is taken as [5]

$$\rho_i(\vec{r}_1,\vec{r}_2) = \left(\frac{Z^3}{\pi}\exp(-Z(r_1+r_2))\right)^2$$

with effective nuclear charge $Z = 1.7$.

The choice of the final detector state in form $\rho = 1$ corresponds to total transition probability to all inelastic channels including excitation and ionization processes. Separation of ionization process in case of strong field considered in [4] is inapplicable in case of weak field since there are no classical paths for electron, which correspond to transition from bound state to ionized one (except autoionization channel in multielectron system). Photo-ionization in weak field is quantum effect. However it can be taken into account since formulas (1), (2) contain phase function – interaction integral *SI*. For separation of ionization process we apply the scheme used in [3], based on restriction of initial electron's position radius.

Now let us consider the choice of the functional $\tilde{S}$, producing phase paths. In case of strong field photo-ionization it is natural to use the choice close to the total action $S$ including interaction of an atom with a field. But in case of weak field it can be used Hamiltonian action $S_0$ for an atom without interaction. This choice significantly simplifies calculations since requires only single set of paths for all values of carrier frequency $\omega$.

As is well known, atoms containing two or more electrons are dynamically unstable to autoionization in purely classical mechanics. It is, therefore, difficult to classically simulate multielectron phenomena which occur over times greater than the autoionization time, which is typically a few femtoseconds. To solve the problem it can be used stabilization of the classical multielectron atom by means of some modification of internal atomic interactions. One of modification scheme is used in FMD method [6]. In this work we modified Coulomb potential by means of regularization in zero point

$$\frac{1}{r} \;\rightarrow\; \frac{1}{\sqrt{r^2+\varepsilon^2}}$$

with parameter $\varepsilon = 0.6$ for electron-electron interaction and $\varepsilon = 0.2$ for electron-nuclear interaction. The functional $\tilde{S}$ was chosen as Hamiltonian action with regularized Coulomb potential. Such regularization was sufficient for obtaining the stabilization time larger than the observation time $t - t'$. The last one is assumed to be much greater then pulse duration $t - t' >> \tau$.

Integration over initial position $q_0$ in formulas (1), (2) were performed by means of Monte-Carlo method.

Let's consider calculation results for helium photo-ionization total cross section in weak laser field. Fig. 1 shows cross section $\sigma$ dependence on carrier frequency $\omega$. The results are obtained for photo-pulse duration parameter $\tau = 10$ (actual duration is about $3\tau$).

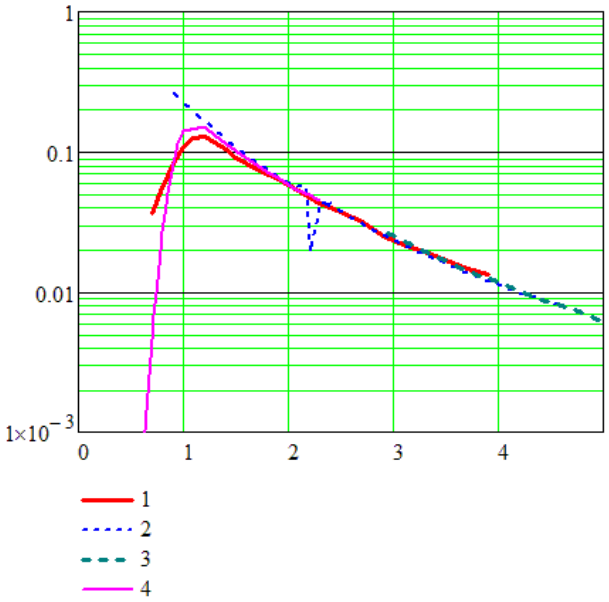


Fig. 1 Helium photo-ionization total cross section $\sigma$ dependence on electric field carrier frequency $\omega$. All values are in atomic units. Lines: 1 – this work; 2 – [7]; 3 – [8]; 4 – TDPT

The results (line 1) are compared with experimental [7] (line 2) and theoretical [8] (line 3) works and with TDPT (time dependent perturbation theory) calculations (line 4). The agreement is rather good. Note that experiment [7] is made with continuous photo-pulse and reproduce a resonance feature on cross section dependence on light frequency, possibly associated with autoionization process. We use shot photo-pulse and all structure on our curve is smoothed within spectral interval about $\Delta\omega \sim \frac{1}{\tau}$.

## IV. Conclusion

The trajectory method, developed in our earlier works, has been tested on calculation of total cross section of helium photo-ionization in weak laser field. This method enables simple estimation of total ionization probability (or cross section) without integration of differential one. It is relatively easy for implementation and allows gaining results in good agreement with other works.

There is a significant difference of probability evaluation using classical path calculations and our method. It is distinct in computing probability in a weak and short field, when there are no classical paths for electron, which correspond to transition from bound state to ionized one (except autoionization channel in multielectron system). Photo-ionization in weak field is quantum effect. Nevertheless described scheme reproduce perturbation theory results quite well since formulas (1), (2) contain phase function – interaction integral *SI*.

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