Evaluation of photoexcitation and photoionization probabilities by trajectory method

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Synopsis A new trajectory-based method of transition probability evaluation in quantum system is developed. Capabilities of the method are demonstrated on evaluating photo-excitation and photo-ionization probabilities in hydrogen atom under exposure of an ultra-short photopulse, and total photoionization probability in the helium atom.

Trajectory methods have many advantages, for example, they are among methods which account the electron-electron correlations. They are widely used when the direct solution of Schroedinger equation is impossible.

In our works [1, 2] we developed trajectory method of transition probability evaluation in quantum system. Here the new variant of this method, using Weyl symbols of initial and final states is represented. The transition probability w is represented in form

$$w = \frac{1}{\nu}\int W_f(q_l, p_l)\left|\exp(iS_I) - K\right|^2 W_i(q_0, p_0)\,dq_0 dp_0$$

$$K = \frac{1}{\nu}\int \exp(iS_I) W_i(q_0, p_0)\,dq_0\,dp_0$$

where $S_I = -\int V\,dt$ – is integral of the interaction, W_i, W_f – Weyl symbols of initial and final states respectfully, q_0, p_0 – initial point of stationary path in phase space, q_l, p_l – final point, $\nu = (2\pi)^n$, n – is the coordinate space dimension.

The developed method was tested on the processes of photo-excitation and photo-ionization in the hydrogen atom by an ultrashort photo-pulse. Also we calculated total ionization crossection in helium atom.

For example, photoexcitation probability dependence on electric field carrier frequency ω for transition between the states 1s $\rightarrow$ 2p in hydrogen atom is shown in figure 1 for the field strength $E = 0.01$ and duration $\tau = 6$. Line 1 represents this method, line 2 – time-dependent perturbation theory. All values are in atomic unit system.

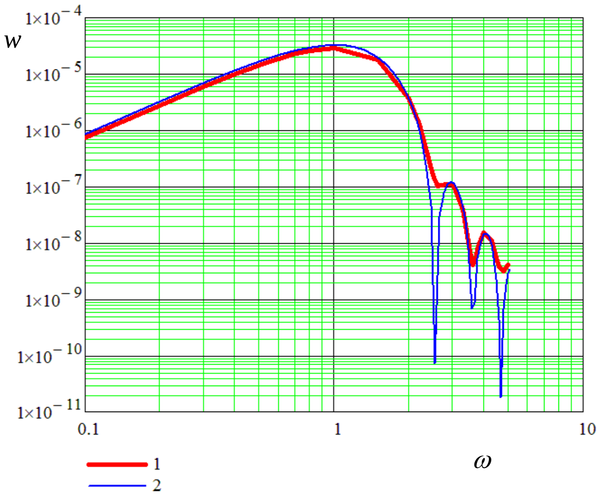

Figure 1. Photoexcitation probability dependence on field carrier frequency ω (atomic units).

The agreement with reliable theoretical results as well as with experimental results are rather good. The method works in wide range of interaction magnitudes. Method is especially relevant to solve the problems in ultraintense and ultrashort laser fields such as calculation of multiphoton multiple photoionization probabilities.

References

[1] Bichkov A.B., Smirnov V.V. 2013 *J. Phys. A: Math. and Theor.* **46** 015303

[2] Bichkov A.B., Smirnov V.V. 2013 *Laser Phys.* **23** 055302

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