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Single hydrogen like atom ionization by ultrastrong laser field: Non-perturbative approach

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Abstract

We develop the method, by which we solve the problem of ionization of single atom exposed to superatomic laser field. Matrix element of ionization transition yields new selection rules. Dependency of ionization rate on the field amplitude is compared with Keldysh formula. Cut-off frequency dependence from field amplitude is obtained.

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1. Basic statements of the theory

In paper [1] new non-perturbative theory of atom–field interaction was proposed. It is based on the following identical transformation of atom + field Hamiltonian:

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+U\right]\psi=V^{-1}\left[\frac{\vec{p}^2}{2m}+U\right]V\psi, \quad (1)$$

where

$$V=\exp\left(-\frac{ie\vec{A}\vec{r}}{\hbar c}\right). \quad (1a)$$

This theory was already applied in the papers [2,3] to the study of some specific features of ionization processes, dipole forbidden harmonics generation, and supercontinuum generation. An important feature of the obtained equation is that neither external field amplitude ratio to the interatomic field strength, nor inverse of it appears to be a small parameter of the problem. At the same time it is seen that the evolution operator V accounts for the multi-quantum processes of the arbitrary order. As shown in [3] the problem analysis comes to the following equation

$$i\frac{da_l(k,t)}{dt}=\sum_n\sum_m V_{km}^{-1(l)}\omega_m V_{mn}^{(l)}a_{nl}(t)+\sum_m\sum_p\int d\mu\, V_{km}^{-1(l)}\omega_m V_{m\mu}^{(p)}a_p(\mu,t)+\text{direct intercontinuum transition items}, \quad (2)$$

and analogous equation for discreet bound coefficients where

$$\psi=\sum_n a_{nl}(t)u_{nl}(\vec{r})+\int dk\, a_l(k,t)u_{kl}(\vec{r})$$

and $u_{nl}(\vec{r})$ are the free atom eigenfunctions. Notice that the matrix elements of evolution operator V are calculated with the help of the free atom eigenfunctions. We consider here summation for periodic indexes that correspond to discreet state and quasi-states of the continuum range of the spectrum that are governed by energy conservation law.

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2. Selection rules

The hydrogenic wave functions of the continuous spectrum are [4]

$$\Psi_k = \frac{C_{kl}}{(2l+1)!}(2kr)^l e^{-ikr} F\left(\frac{i}{k}+l+1, 2l+2, 2ikr\right) \times P_l(\cos\theta) = R_{kl} P_l(\cos\theta), \tag{3}$$

where

$$C_{kl} = 2k e^{\frac{\pi}{2k}} \left|\Gamma\left(l+1-\frac{i}{k}\right)\right|,$$

$F(\frac{i}{k}+l+1, 2l+2, 2ikr)$ is the confluent hypergeometric function, $\Gamma(l+1-\frac{i}{k})$ is the gamma function, $P_l(\cos\theta)$ is the Legendre polynomials. Note, that each level is infinitely degenerated with respect to the orbital number. Let us consider ionization from the ground state of hydrogen like atom. The exact calculations show that the matrix elements of the evolution operator between the continuous spectrum states are equal to zero. Thus, we need only in the following matrix elements

$$V_{1s\to k}^{(l)} = \sqrt{\pi}\int 2e^{-r} e^{i\frac{\Omega}{\omega}T(t) r\cos\theta} \Psi_{kl}(r) r^2 \sin\theta\, dr\, d\theta, \tag{4}$$

where Ω is the Rabi frequency, ω is the carrier frequency of the laser field, and $T(t) = \sin(\omega t) e^{-(t-t_0)^2/\tau^2}$. The integral over the angular variables can be easily calculated with the help of the explicit form of Legendre polynomials

$$P_l(\cos\theta) = \frac{1}{2^l l!}\frac{d^l}{(d\cos\theta)^l}\left(\cos^2\theta - 1\right)^l.$$

The result of calculations takes form of the following power series

$$V_{1s\to k}^{(l)} = 2\sqrt{\pi}\int_0^\infty dr\, r^2 R_{kl} e^{-r} \sum_{n=l}^{\infty}\left(\frac{\Omega}{\omega}T(t) r\right)^n \times \frac{(1-(-1)^{n-l-1})}{2^n \Gamma(\frac{1}{2}(3+l+n))\Gamma(\frac{n-l}{2}+1)}. \tag{5}$$

It should be reminded here that, according to the standard selection rules, the transition from the ground state of the hydrogen-like atom is allowed only to the finite state of $l = 1$. It is prescribed by the matrix elements of the Hamiltonian of the electro-dipole interaction. The integration over the angular variables shows that the terms of the series (5) is exactly equal to zero at $n < l$, therefore the series (5) includes only terms with $n \geqslant l$. It is seen from Eq. (5) that the terms of the series is equal to zero at $n - l = 2p + 1$, where p is an integer. Therefore the selection rules, generalized for account of the ATI transitions of the arbitrary order, means that (i) $n - l \neq 2p + 1$, where $p \in \mathbb{Z}$, (ii) $n \geqslant l$. It should be noted that in the limit of weak field the above selection rules come to that well known in dipole approximation.

Summing the series, we obtain

$$V_{1s\to k}^{(l)} = 2(2\pi)^{3/2}(2k)^{l+1} e^{\frac{\pi}{2k}} \frac{|\Gamma(l+1-\frac{i}{k})|}{2^l(2l+1)!}\sqrt{\frac{\omega}{\Omega}\frac{1}{T(t)}} \times \int_0^\infty dr\, r^{l+\frac{3}{2}} e^{-r} e^{-ikr} F\left(\frac{i}{k}+l+1, 2l+2, 2ikr\right) \times J_{\frac{1}{2}+l}\left(\frac{\Omega}{\omega}T(t) r\right), \tag{6}$$

where $J_{\frac{1}{2}+l}$ is the spherical Bessel function. Integral (6) can be useful for an analysis of space patterns, but for the investigation of integrative features gives not much. Hence in the expression (5) let us make a calculation of the integral before summation of the series, which is acceptable due to the convergence of both. Then we get the following expression

$$V_{1s\to n}^{(l)} = 2(\pi)^{3/2}\left(\frac{\Omega}{\omega}T(t)\right)^n \frac{(1-(-1)^{n-l-1})(n+l)!}{2^n\Gamma(\frac{1}{2}(3+l+n))\Gamma(\frac{n-l}{2}+1)} \times \left(2\sqrt{-E+n\hbar\omega}\right)^{l+1} \frac{|\Gamma(l+1-\frac{i}{\sqrt{-E+n\hbar\omega}})|}{(2l+1)!} \times e^{\frac{\pi}{2\sqrt{-E+n\hbar\omega}}}\left(\frac{1}{i\sqrt{-E+n\hbar\omega}+1}\right)^{n+l+1} \times F_2\left(\frac{i}{\sqrt{-E+n\hbar\omega}}+l+1, n+l+1, 2l+2, \frac{2i\sqrt{-E+n\hbar\omega}}{i\sqrt{-E+n\hbar\omega}+1}\right), \tag{7}$$

where F_2 is the hypergeometric function of the second order, and n is the number of absorbed photons. In (7) we have use of energy conservation law in the following form $\frac{\hbar^2k^2}{2m} = n\hbar\omega - E$, where E is the atomic ionization energy, and applied the formula

$$\sum_{n=l}^{\infty} f(n)g(k)\delta_{nk} = f(k)g(k).$$

Note that in such approach we summate the whole series and not some first harmonics, which allows us to declare non-perturbance.

Eq. (7) shows that the number of the quasi-energy states, having non-zero matrix elements with the ground state, is finite even in the superstrong laser field. For example, as it is seen from Fig. 1, only first 20 quasi-energy states have the non-zero matrix elements at $\frac{\Omega}{\omega} \approx 5$ (the ratio of the laser field strength to the intra-atomic field strength is equal approximately to 5). Thus, Eq. (7) enables us to determine the number of the quasi-energy states that we should take into account at a given laser filed amplitude. As a result we can optimize significantly the procedure of the numerical solution of the coupled set of Eqs. (2).