Above-threshold ionization of one-active electron atomic systems in the x-ray regime: a non-perturbative treatment

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Synopsis We study in the framework of the nonrelativistic semiclassical approach the ionization of simple atomic systems by intense XUV and soft-X pulses of short durations. We present and discuss photoelectron distributions for various working conditions, highlighting in particular the increasing importance of the non-dipole effects for pulses of few cycles and intensities beyond the value $I_0 \approx 3.5 \times 10^{16}$ W/cm$^2$.

We investigate through nonrelativistic "exact" calculations the ionization of atomic systems with one electron by linearly polarized short pulses of radiation in the spectral range XUV and soft-X. The computations involve i) the numerical integration of the time-dependent Schrödinger equation, done in our case in the interaction representation with eigenstates of unperturbed Hamiltonian constructed in terms of B-spline functions [1], followed by ii) the extraction of the photoelectron distributions from the wave function at the end of interaction of the atom with the radiation pulse.

Our numerical simulations cover the range of radiation intensities comparable to $I_0$ and higher, and of pulse durations from a few cycles to tens of cycles. For the energies of the photons we consider the interval between 100 eV and 5 keV, the corresponding wavelengths ranging from $\approx 37$ a.u. to $\approx 0.75$ a.u., thus becoming comparable with the atomic "dimensions". In order to take into account this fact we have adopted an approximate treatment of the nonhomogeneity of the radiation pulse, similar in essence with that described in [2]. The corresponding approximate Hamiltonian contains corrections of the first order in $\alpha \approx 1/137$ to the Hamiltonian in electric dipole approximation.

We studied how the ionization features as function of the radiation pulse parameters - wavelength, peak intensity and duration. For longer pulse durations and lower intensities the nonrelativistic electric dipole approximation is still acceptable at the level of photoelectron energy spectrum. Assuming the atom is initially in the ground state, the deviation between the results obtained in this approximation and the exact ones is less or of the order $\approx 5\%$ for the whole range of radiation frequencies considered.

However, reducing the pulse duration and/or increasing the radiation intensity, the nondipole effects begin to play a more significant role.

For conditions mentioned above we present and discuss photoelectron distributions, integrated or analyzed in energy, electron emission direction or angular momentum. We compare them with the same type distributions in dipole approximation in order to understand how relevant are the retardation effects.

We also explored the atomic response in two special circumstances, both having a potential impact over the quality of dipole approximation for a given XUV pulse. The first one refers to the modification of the results with the atomic number. In particular, for low values of this parameter, we examine the deviation of the results from a well-known scaling law in $Z$, valid in the case of dipole approximation and for Coulomb potential. A second situation considered regards the ionization from excited initial states, for which we present some preliminary results. The motivation of the study, in both cases, is related to the possibility to modify the spatial extension of the atom.

This work has been supported by CNCSIS-UEFISCSU, project number 488 PNII-IDEI 1909/2008, and has benefitted from scientific cooperation open by the COST action CM0702.

References

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