Simulation of High Harmonic Generation in Xenon Based on Time-Dependent Density-Functional Theory

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The high harmonic generation (HHG) of intense laser pulses is one of the most well-known phenomena of strong-field physics, which is of great interest in terms of numerous applications [1]. The physical mechanism of HHG is qualitatively explained in the framework of a three-step scenario [2]. At the first step, atoms or molecules are ionized by an intense field. At the second step, the electric field accelerates the free electrons in the continuum. At the third step, the electrons recombine with the emission of high-energy photons in a wide energy range. In the first and third steps, the multielectron dynamics associated with the motion of various electrons in an atom or molecule can significantly affect the form of HHG spectra [3-8]. An example of the significant influence of multielectron effects at the final step is the giant enhancement of HHG yield in xenon [4-7].

In this work, we study the HHG in xenon based on the time-dependent density functional theory for the first time analytically and numerically [8]. For numerical calculations, we use the developed computer code for the solution of the three-dimensional time-dependent Kohn-Sham equations for atomic orbitals taking into account the interaction of electrons with the laser pulse, nucleus, and each other. Our numerical code allows considering the dynamics of all subshells on the 4th and 5th atomic shells of the Xe atom. We show that the perturbation of the electron-electron interaction potential induced by recolliding photoelectron wavepacket originated from the $5p_0$ orbital leads to the collective oscillations of all orbitals on the 4th shell closely localized in space and strongly interacting with each other. At the enhancement region and higher frequencies, HHG is influenced not only by the $4d$ subshell but also by the other $4p$ and $4s$ subshells on the 4th shell. The high accuracy of the obtained results is confirmed by comparing the calculated HHG spectra with experimental results [4] and an analytical parameterization of the HHG yield.

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