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Numerical Simulation of Ion-Based Water-Window Harmonic Generation in Laser-Irradiated Gases

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High-harmonic generation (HHG) induced in laser-irradiated atomic or molecular gases is an important method to generate water-window soft X-ray. The focused laser pulse ionizes the gas medium, and the released electrons undergo the acceleration and recombination processes to emit short-wavelength photons [1]. The figure of merits to characterize the performance of HHG are the cutoff photon energy and the conversion efficiency.

The cutoff photon energy of HHG E_c can be derived that $E_c = I_p + 3.17U_p$, where I_p is the ionization potential, and U_p is the ponderomotive energy. In order to increase E_c, e.g. water-window X-ray range, ion species is a better HHG emitters. Ion has higher ionization potential than atom, cause the higher cutoff energy. In addition, with higher I_p, the ions can only be ionized under a higher laser intensity, which increase U_p. Based on the above conditions, we choose He as our neutral gas target, and generate the high harmonic by He and He^{1+}.

The conversion efficiency of HHG is mainly determined by the phase-matching condition of the generation process. It is determined by four mechanisms, i.e., neutral gas dispersion, plasma dispersion, geometrical phase shift (Gouy phase shift), and intensity-dependent dipole phase variation. Moreover, using a shorter wavelength driving laser can also enhance the conversion efficiency, since the single-atom response scales with $\sim\lambda^{-6}$ between interactions of different laser wavelengths with the same atom [2]. However, in the highly-ionized plasma regime, which represents high density HHG source, plasma dispersion is hardly to be balanced. Therefore, the phase-matching condition is difficult to be achieved, such that generation of high efficiency HHG at short wavelength becomes a big challenge.

In this paper, we perform a numerical simulation of the ion-based HHG. We found that phase-matching condition can be achieved for water-window x-ray emission driven by 405-nm femtosecond pulses. We first apply the 3+1-dimensional hybrid advective-diffusion electromagnetic (EM) envelope equation with cylindrical symmetry, together with Keldysh's optical-field ionization model, to resolve the propagation of the driving pulse in a He gas target. The moving-window algorithm is adapted while solving the equation, as shown in Figure 1. Then we can have the ion/electron density distributions and calculate the phase-matching condition and the HHG yield.

The driving pulse specification is optimized to 16.5-mJ energy, 405-nm wavelength, and 30-fs duration. It is focused to a waist radius of 30 μm at z = 0. The Helium gas is located between $z = 7$ mm and $z = 10$ mm, with a uniform density distribution $1.8 \times 10^{17}\ \mathrm{cm}^{-3}$. The resulted laser intensity, gas density, and electron density in *z*-*r* space are shown in Figure 2. The phase-matching condition is achieved for the 93rd-order harmonic (4.35 nm) on the propagation axis (*r* = 0), as shown in Figure 3. The 4.35-nm output yield generated through the processes of $\mathrm{He} \rightarrow \mathrm{He}^{1+} \rightarrow \mathrm{He}$ and $\mathrm{He}^{1+} \rightarrow \mathrm{He}^{2+} \rightarrow \mathrm{He}^{1+}$, as well as the total HHG yield, are accumulated constructively within the entire interacting region.

References
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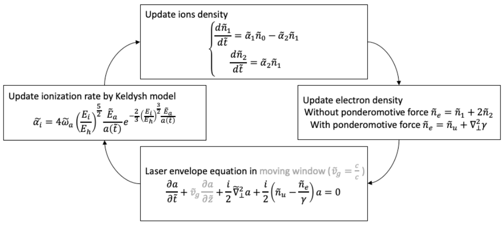

Figure 1. Schematic illustration of the numerical algorithm. $\tilde{n}$ is the normalization density and a is the normalization wave vector amplitude.

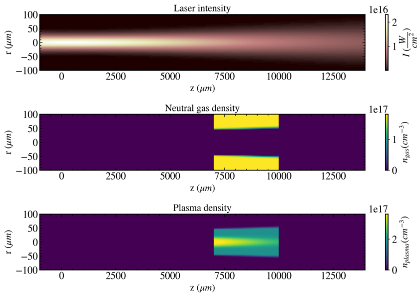

Figure 2. Simulation results show spatial profiles of laser intensity, helium gas density and electron density in z-r space.

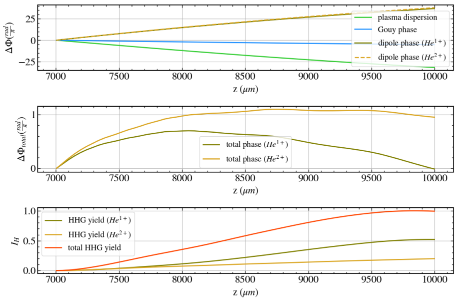

Figure 3. Phase matching condition and HHG yield varies along the propagation axis ($r = 0$).