Spatial distribution on high-order-harmonic generation of an H_2^+ molecule in intense laser fields

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Synopsis High-order-harmonic generation (HHG) for the H_2^+ molecule in a 3-fs, 800-nm few-cycle Gaussian laser pulse is investigated by solving the time-dependent Schrödinger equation. The spatial distribution on HHG is demonstrated and the results present the recombination process of the electron with the two nuclei. And there is little possibility of the recombination of the electron with the nuclei around the origin z = 0 a.u. and equilibrium internuclear positions z = ±1.3 a.u.. The electron-nuclear wave packet and ionization probability are investigated to explain the physical mechanism.

High-order-harmonic generation (HHG) via laser-matter interaction has been intensively studied in recent years because of its applications in generating isolated attosecond pulses [1]. The attosecond pulses are significant for probing, for example, nuclear dynamics and photoelectron wave packets [2].

In this work we investigate the spatial distribution on HHG of the H_2^+ molecule in an intense laser field, the dipole acceleration distribution in each electronic coordinate can be written as [3, 4].

$$d_A(z,t) = -\int_0^R \psi^*(z,R,t)\left(\frac{dV_C(z,R)}{dz} + (1+\frac{m_e}{2m_p+m_e})E(t)\right)\psi(z,R,t)dR$$

By using the dipole acceleration distribution in each electronic coordinate, the contribution of each electronic coordinate on HHG can be demonstrated as shown in Fig. 1, in which the horizontal axis represents the harmonic order, the vertical axis represents the electronic coordinate, and the depth of the color represents the intensity of the harmonics.

The results show that if the electric field reaches its negative peak, the electron is ionized along the positive-z direction. When the laser reverses, the electron slows down until it is pulled back and the contribution to the HHG mainly comes from the recombination of the electron with the nucleus along the positive-z direction. Meanwhile, if the electric field reaches its positive peak, the electron is ionized along the negative-z direction. When the laser reverses, the electron slows down until it is pulled back and the contribution to the HHG mainly comes from the recombination of the electron with the nucleus along the negative-z direction. We also illustrate that there is little possibility of recombination of the electron with the nuclei around the origin z = 0 a.u. and equilibrium internuclear positions z = ±1.3 a.u. from the spatial distribution of the HHG spectra. The underlying physical mechanism can be well understood by the three-step model and the time-dependent electron nuclear wave packet.

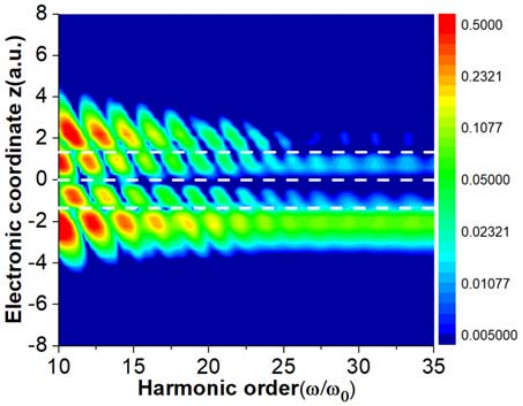

Figure 1. Spatial distribution of the HHG spectra as a function of the electronic coordinate and harmonic order for the 1D H_2^+ molecule in the Gaussian laser field. The white dashed lines indicate the positions of the electronic coordinate at the origin z = 0 a.u. and the equilibrium internuclear distance z = ±1.3 a.u., respectively.

References

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