High-Order Harmonic Generation of hydrogen molecule ions in a large internuclear distance*

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Synopsis We study high-order harmonic generation (HHG) by solving a two-dimensional time-dependent Schrödinger equation (TDSE) for a hydrogen molecular ion H_2^+. A double plateau structure is detected in harmonic spectra, the wavelet time-frequency analysis and an extended semiclassical analysis show that the width of the first plateau can be used to estimate the internuclear distance of H_2^+.

The HHG of H_2^+ with internuclear distance R=14 a.u. was obtained by solving 2D TDSE using the time-dependent Crank-Nicolson method [1]. The time-frequency analysis by means of the Morlet transform [2] and a generalized 2D semiclassical approach with the inclusion of the molecular potential [3] are performed to probe the features of the HHG.

Figure 1 shows the HHG spectra of H_2^+ driven by a 1600-nm laser pulse with the peak intensity $I = 2.14\times10^{14}\,\mathrm{W/cm^2}$. It is clear that a double platform structure can be found in the HHG spectra. The cutoff of the first plateau is equal to 37, which corresponds with the energy of classical calculation eE_0R (E_0 is the intensity of laser field) [4]. That is to say the first plateau of the HHG is due to the electron motion by migrating from one nucleus to the other.

Figure 2 shows time-frequency analysis spectra and the semiclassical energy of H_2^+ as a function of return time of the electron. First, the semiclassical energy is in good agreement with those of the time-frequency spectra of the HHG. Second, in Fig.2(a) and Fig.2(b), the trajectories that lie below the harmonic 40 suggest the migratory motion of electron between one nucleus and the neighboring one. Thus, we can estimate the internuclear distance of the diatomic molecule by the width of the first plateau.

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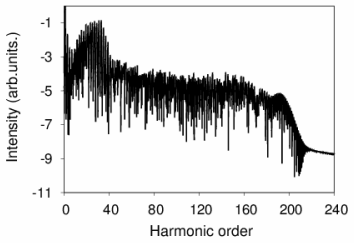

Figure 1. HHG spectra of H_2^+ driven by a 1600-nm laser pulse.

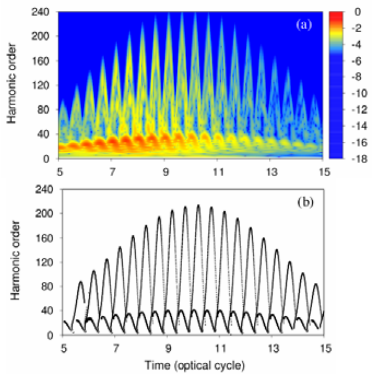

Figure 2. (a) Wavelet time-frequency analysis of HHG spectra; (b) the semiclassical return energy map.

References

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