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Dynamical origin of below-threshold harmonic generation of diatomic molecules

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Synopsis We present an *ab initio* quantum study of below-threshold harmonic generation (BTHG) from H_2^+ molecules in the presence of an intense laser field by solving the time-dependent Schrödinger equation accurately in space and time. We find that multiple channels contribute to BTHG of H_2^+ molecules, which are related to the electron driven initially at specific time of the laser pulse from one nuclear core to another nuclear core or back to the parent core itself. The distinct contributions of these channels are distinguished by using a novel synchro squeezing time-frequency analysis.

High-order harmonic generation from atoms and molecules is a fundamental strong-field process attracting much attention due to its applications in ultrafast science and technology, such as the generation of attosecond pulse. The attosecond pulse further allows the direct detection and control of the electronic dynamics in atoms and molecules system. Recently considerable attention has been paid to the harmonic generation below the ionization threshold, where it is a potential way to produce vacuum-ultraviolet source. Most previous studies focused on the atomic system in below-threshold harmonic generation (BTHG) [1]. For the molecular systems, due to the presence of the extra internuclear degree of freedom [2], the BTHG becomes more complex.

In Figure 1(a), we present the below-threshold harmonics of H_2^+ molecular ions in an intense laser field. The black vertical dashed lines indicate the ionization threshold of the initial state marked by I_p of H_2^+ molecules. Figure 1(b) shows the Wavelet transform of time-frequency spectra of the BTHG. It is clearly seen that the Wavelet time-frequency spectra of H_2^+ molecules below ionization threshold are subject to some obscure features due to the broadband width in time-frequency distribution. However, as shown in Figure 1(c), the advantage of the synchrosqueezed transform [3] as comparing to other widely used the time-frequency transform is its capability to generate sharper and clearer time-frequency distributions which then allows to identify the individual role of multiple channels below the ionization threshold in time-frequency domain.

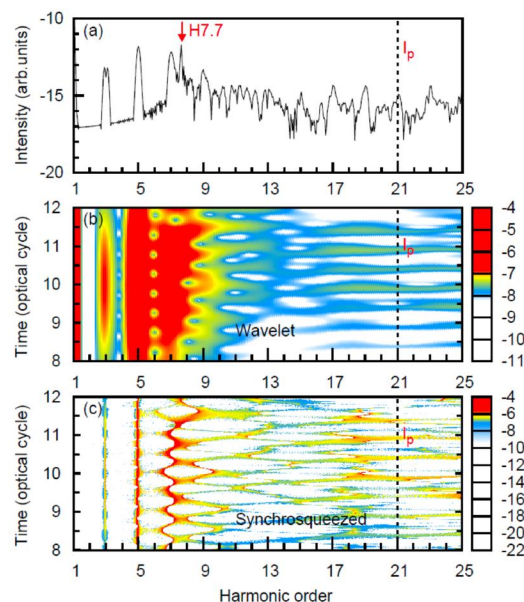


Figure 1. BTHG of H_2^+ molecules and time-frequency analysis by the Wavelet and Synchrosqueezed transform, respectively. The red arrow indicates that the resonant peak is located at the harmonic order 7.7 (H7.7).

Acknowledgments

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