Theoretical study of terahertz generation from atoms and aligned molecules driven by two-color laser fields

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***Abstract*—We study the generation of terahertz (THz) radiation from atoms and molecules driven by an ultrashort fundamental laser and its second harmonic field by solving time-dependent Schrödinger equation. The simulations show that the initial wave-packet and its subsequent acceleration in the laser field, and rescattering with long-range Coulomb potential play key roles on THz generation. We also present the dependence of the optimal phase delay and yield of terahertz radiation on the laser intensity, wavelength, duration, the ratio of two-color laser components, and against the molecular alignment.**

I. Introduction

Among THz generation techniques, laser air photonics is capable of generating THz field strength greater than 1 MV/cm with bandwidth of over 100 THz through plasma formation by laser ionized gaseous medium. But its mechanism of THz generation turns out be complicated involved of wave propagation, plasma formation, oscillation and collision [1-4,7].

In the present investigation, we explore further the effects of atomic potential and other laser parameters on the generation of THz for both a hydrogen atom and a model H_2^+ molecule interacting with two-color pulses.

II. Results

We first examine in details how the THz yields depend on various of parameters of the two-color laser pulses, especially the optimal phase-delay (OPD) and optimal THz yield that maximizes (optimize) the THz yields (OTY). When the atomic potential is the long-range Coulomb potential, for either 1D, 2D or 3D calculations (Fig.1a), the optimal phase follows the same trend that varys from 0.9π to 0.6π as increasing laser intensity. The intensity dependence of the OPD indicates that different ionization mechanism are involved. As the laser intensity increases, the ionization mechanisms varies from multi-photon ionization to tunneling ionization and over-the-barrier ionization. The dominated mechanisms of THz generation are from four-wave-mixing, rescattering currents of soft-recollision between ionized electron with atomic core [3], to photocurrent model without Coulomb potential [2], respectively. The dependence on the intensity ratio of both the OPD (Fig.1b) and OTY (Fig.1e) are consistent with laser-assisted soft-collision model presented in [4], and the OTYs are scaled as power of the intensity ratio, which is consistent with the experiment [5]. As the laser wavelength increases, the OPDs obtained from TDSE shift from 0.8π to 0.5π (Fig.1c). This variation might be rationalized that the wave packet is more diffused during each cycle for the longer wavelength, and the soft-recollision with atomic nuclear plays less rule. However, the discrepancy of OTY's wavelength scaling between numerical (Fig.1f) and experimental data [5] needs further investigation in the future.

Next, we focus on THz and HHG generation dependence on both molecular alignment angle θ and molecular potential. The total OTYs, dominated by parallel component to laser polarization, take maximum at $\theta = 0°$ and minimum at $\theta = 90°$ respectivley (Fig.1g), which closely assembles the angular dependence of the ionization probability and has been confirmed by experiment [6]. The maximum variation of OPDs is found less than 0.1π (Fig.1h-i). Although this variation, converting into a time delay of 67 attoseconds, is small, it indeed indicates that the molecular potential plays a role in the generation of THz waves. Furthermore, it clearly demonstrates that THz yields can be used to gauge the harmonic yield to gain the two-center interference information of HHG. The phase-delay dependence of THz generation can be used to probe the modulation of harmonics as well.

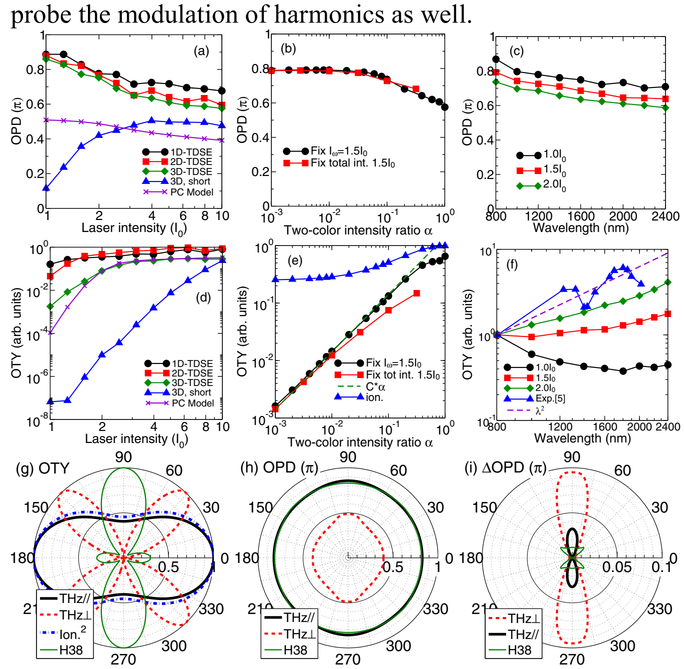

Fig. 1 (Color online) The optimal phase delay and terahertz yield dependence on laser intensity (a,d), two-color intensity ratio (b,e), wavelength (c,f), and molecular alignment (g,h). (i) the OPDs difference between molecular alignment angles and parallel alignment.

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