

Angular Harmonic Dependence from a 3D-H₂⁺ Molecular Ion

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ABSTRACT

The time-dependent Schrodinger equation of a H₂⁺ molecular ion in the presence of a linearly polarized laser field is numerically solved by means of a split-operator parallel code. The electron, driven by the laser electric field, emits electromagnetic radiation whose HHG spectrum (shown in Figure 1) can be finely controlled by changing the angle between the laser electric field and the molecular axis. The numerical results confirm that the structure of the spectra strongly depends on this angle. In particular the correlation between the laser orientation (with respect to the molecular axis) and the intensity of various harmonic peaks are displayed in Figure 2.

THE CONTEST

High Harmonic Generation (HHG) arises from the nonlinear response of the electron wave function to intense laser fields: an electron is driven by a strong laser field away from its parent atom or molecule, propagates in the field, and returns to the parent ion with the emission of high-energy photons. The emitted radiation can be used in the production of UV or XUV pulses and to probe the electron dynamics; it carries information on the emitting source allowing a tomographic image of atoms and molecules.

THEORETICAL MODEL

The temporal evolution of the physical system is obtained through the numerical solution of the Time-Dependent Schrodinger Equation (TDSE) with fixed nuclei:

$$H\psi(\mathbf{r},t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r},t)$$

where

$$H = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}, \mathbf{R}_1, \mathbf{R}_2) + W_E \equiv \text{Hamiltonian operator}$$

\mathbf{r} \equiv electronic coordinate

\mathbf{R}_i \equiv position of i^{th} nucleus

$$U(\mathbf{r}, \mathbf{R}_1, \mathbf{R}_2) = -\frac{e^2}{|\mathbf{r} - \mathbf{R}_1|} - \frac{e^2}{|\mathbf{r} - \mathbf{R}_2|} \equiv \begin{cases} \text{electron-nuclei interaction} \\ \text{energy operator} \end{cases}$$

$$W_E = -e\mathbf{r} \cdot \mathbf{E}(t) \equiv \text{electron-laser interaction energy operator}$$

RESULTS

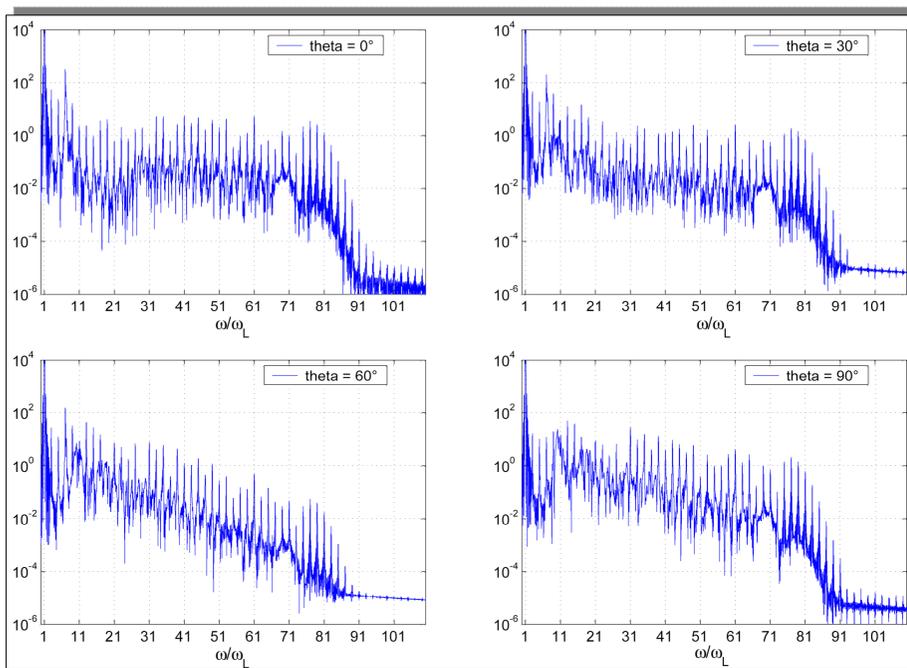


Fig.1: Full Emitted Spectra for different molecular alignment angles

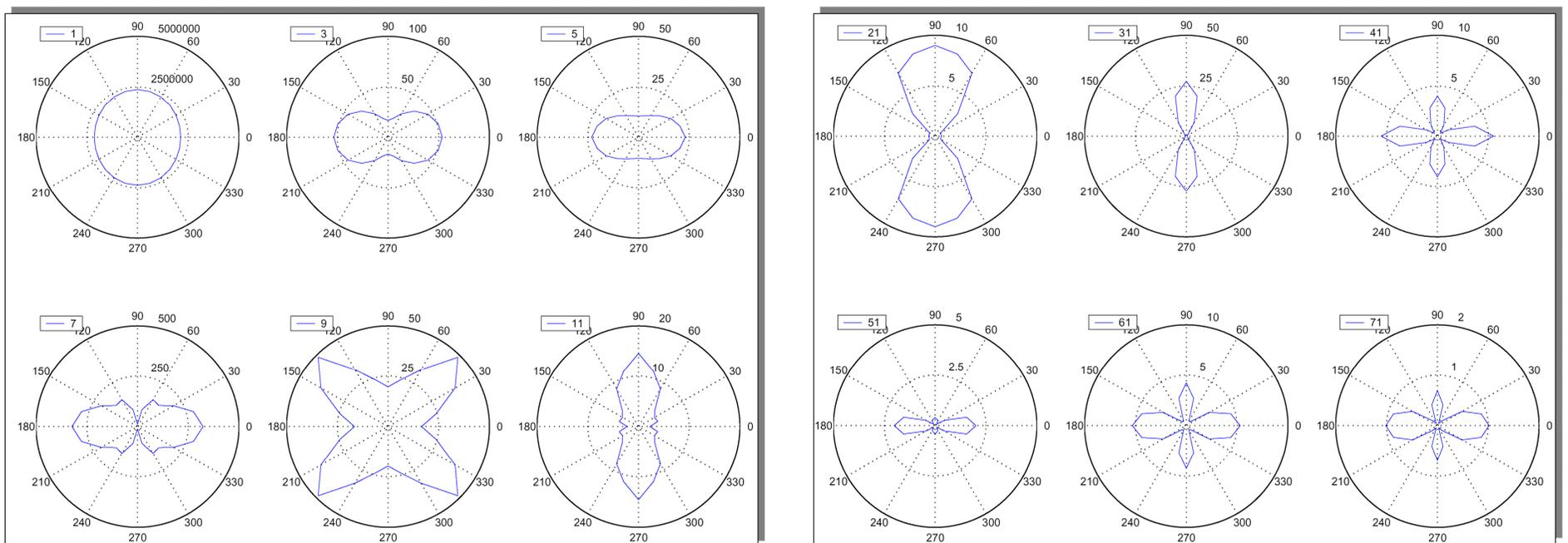


Fig.2: Some harmonic peaks as a function of different molecular alignment angles

CONCLUSIONS

The numerical computations have shown that the emitted spectrum is strongly modified if the angle between the laser electric field and the molecular axis is changed. These findings suggest that the knowledge of the angular profile of the emitted spectra can be used to investigate the molecular alignment process. Moreover it has been proposed to use the angular dependence of the HHG as a tool to obtain real images of molecular bonding orbitals.

Acknowledgments

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