MACROSCOPIC SIMULATION OF NEAR-THRESHOLD HIGH HARMONIC GENERATION USING MICRO-SCOPIC TDSE/TDDFT CALCULATIONS

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Modelling strong-field induced radiation near the ionization threshold requires careful treatment of excited state dynamics. Solution of the time dependent Schrodinger equation (TDSE) provides accurate data in this regime, but the computational time needed prohibits direct calculation of the macroscopic response (e.g., from a gas jet) due to the range of intensities to be considered. We apply a method of interpolation of (precalculated) TDSE results as a function of laser intensity at a given wavelength to simulate the macroscopic propagation of the high harmonic signals using the discrete dipole approximation. This allows investigation of the angular dependence of harmonic and off-harmonic radiation near and below the ionization threshold (see Fig. 1). The method can be extended beyond the hydrogen atom through the Single Active Electron (SAE) approximation or Time Dependent Density Functional Theory (TDDFT). Results for the helium atom (SAE) and N_2^+ molecule (TDDFT) will be presented.

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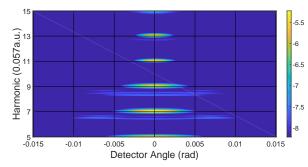


Figure 1: Angle-resolved high-order harmonic spectrum from 5×10^5 hydrogen atoms. Note the difference in structure of harmonic peaks versus off-harmonic lines