Intramolecular interference effects in photoelectron momentum distributions arising due to strong-field molecular ionization

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Synopsis The strong-field phenomenon of multiphoton above-threshold ionization (ATI) in laser-irradiated molecular dimers (H_2, N_2 and O_2) is addressed theoretically within the *velocity-gauge* formulation of *strong-field approximation* under conditions of experiments with a laser field of mid-infrared wavelength ($\lambda \geq 800$ *nm*). Our calculation results demonstrate clear signatures of *intramolecular interference* manifested as pronounced and well-established *interference* minima arising in photoelectron momentum distributions whose form and structure proved to be sensitive to internuclear separation R_0 and spatial orientation of molecular axis.

We report about the results of our theoretical study of strong-field (multiphoton) above-threshold ionization (ATI) in laser-irradiated molecular diatomic species (H_2, N_2 and O_2) under conditions of experiments [1, 2] observing a characteristic (the so-called *two-hump*) structure in longitudinal photoelectron momentum distributions (PMD), which becomes especially prominent using mid-infrared laser wavelengths ($\lambda \geq 800$ *nm*). The problem is addressed within the *velocity-gauge* (VG) formulation of molecular *strong-field approximation* (SFA) [3]. In particular, only the so-called *direct* ATI process is supposed as quite a sufficient underlying physical mechanism solely contributing to the phenomenon under study. Moreover, the *density-functional theory* (DFT) is also essentially exploited here for numerical composition of initial (laser-free) atomic and/or molecular state using the routines of GAUSSIAN-03 code [4].

Our present DFT-SFA based calculation results suggest the *two-hump* form of longitudinal atomic/molecular PMDs similar to those observed in experiments for atomic ionization in the tunneling regime (the value of the *Keldysh parameter* $\gamma \leq 1$). In particular, for the photoelectron emission parallel to the laser field polarization, the calculated molecular PMDs (e.g. for ionization of N_2 see Figure 1) also represent a symmetric sequence of discrete photoelectron peaks in the parallel-momentum distributions with a prominent central minimum between the two symmetrically located and well-extended "horn-like" side-lobes (humps). However, unlike the atomic case, Figure 1 remarkably demonstrates a substantially different form of calculated molecular PMDs (as an envelope of peaks) which is well seen to suggest a presence of two distinct and pronounced minima - each located within a respective (either of two symmetric) hump. In addition, the form and location of these minima proved to be well sensitive to spatial orientation of molecular axis relative to the incident laser field polarization (though quite insensitive to the laser wavelength λ and peak intensity I). The latter feature allows to identify the origin of minima and interpret them as arising due to *intramolecular interference* of multiphoton transition amplitudes corresponding to the photoelectron emission from either of two identical atomic centers of molecular dimer under ionization.

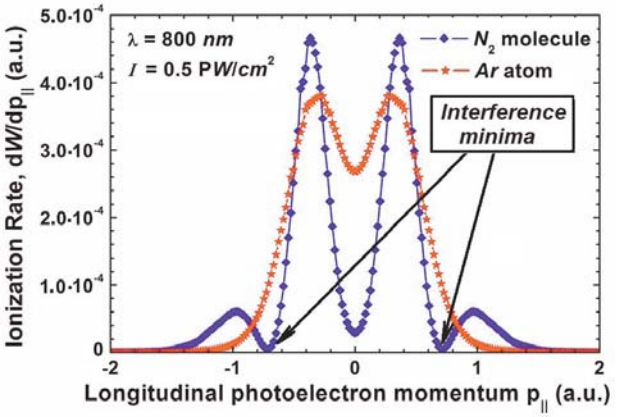

Figure 1. PMDs calculated for ionization of *Ar* atom and N_2 molecule aligned along the polarization of incident laser field of fixed wavelength λ and peak intensity I (as indicated in the picture inset).

References

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