Theoretical Study of Electron-Nuclei Entanglement in Molecular Photoionization

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We are interested here in molecular photoionization where the correlations between the photoelectron and the vibrational dynamics of the ion are likely to create entanglement [2]: the total system can then no longer be written as the product of the two subsystems, which translates into a loss of co- herence in partially resolved measurements. Using simulations on a model molecule inspired by H2, composed of an active electron and two nuclei. We investigate how decoherence manifests in XUV molecular photoemission [3] :

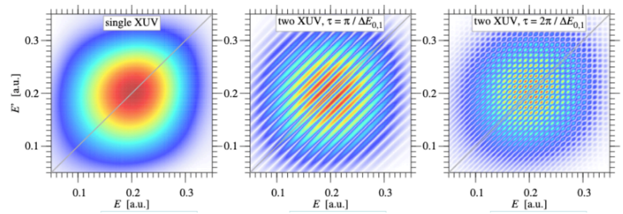

Figure 1: Photoelectron reduced density matrix obtained when ionizing our model molecules with a pair of 21.7 eV pulses with various delays (see also [3])

$$H_2 + \hbar\omega \longrightarrow H_2^+(\nu) + e^-(k). \quad (1)$$

We focus on how this loss of coherence trans- lates into experimental observables and ultimately into their interpretation in terms of ultrafast dynamics. More precisely, we consider the case of molecular RABBIT [4] and mixed-FROG [5] and compare the actual dynamics revealed in time-dependent numerical simulations to the dynamics reconstruct- ed from electron spectra or ion yields « measured » at various levels of resolution. We also study how external parameters (such as the temporal structure of the ionizing field) influence the degree of entanglement.

References

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